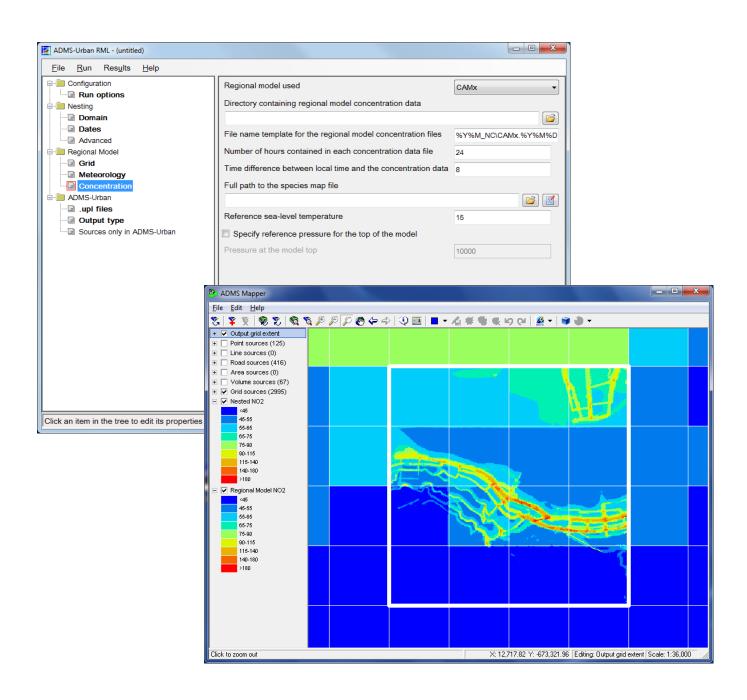


ADMS-Urban Regional Model Link

Automated System for Nesting ADMS-Urban in a Regional Air Quality Model



User Guide

CERC



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User Guide

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Cambridge Environmental Research Consultants Ltd.

3, King's Parade

Cambridge

CB2 1SJ

UK

Telephone: +44 (0)1223 357773 Facsimile: +44 (0)1223 357492 Email: help@cerc.co.uk Website: www.cerc.co.uk

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SECTION 1 Introduction

1.1 About the ADMS-Urban RML system

The ADMS-Urban Regional Model Link (ADMS-Urban RML) is an automated system for nesting the high resolution air quality model ADMS-Urban (McHugh *et al.*, 1997) in a regional air quality model such as CMAQ (Byun and Schere, 2006), CAMx (ENVIRON, 2014) or EMEP4UK (Vieno et al., 2010). The output from the RML system comprises predictions of pollutant concentrations for an urban area, which take into account both regional and local pollutant transport and chemistry effects.

The aim of the ADMS-Urban Regional Model Link system is to combine the complementary advantages of regional and local models to improve the prediction of concentration values for all types of receptors. Regional (usually Eulerian) models contain complex chemistry mechanisms, which can operate over long spatial and temporal scales, and can model the accumulation of concentrations in very low wind speed conditions. The gridded nature of their emissions data and dispersion calculations, however, does not allow them to resolve the high gradients of concentration found in the immediate vicinity of an individual source such as a road. Local (usually Gaussian-type plume) models can represent the fine-scale concentration gradients from explicitly defined sources in detail, but generally only include simplified chemical mechanisms and spatially homogeneous meteorological data, limiting their applicability for receptors far from the source (typically defined as more than 50 km). They are also of limited applicability in very low wind speed conditions.

Nesting a local model within a regional model can allow both the resolution of high concentration gradients close to a source, and the accurate representation of transport and chemistry over larger spatial and temporal scales. The ADMS-Urban RML system combines the regional and local concentrations in such a way as to minimise double-counting of emissions, while remaining computationally efficient and user-friendly. It is an off-line system, meaning that the regional models can be run separately from the local modelling, which allows the use of archived regional model data. Meteorological data from the WRF meso-scale model (Dudhia *et al.*, 2005) is used for both the regional modelling and the local modelling. An overview of the ADMS-Urban RML system is given in Section 1.3 while a technical summary of the concept and implementation of the ADMS-Urban RML system can be found in Section 8.

At present the ADMS-Urban RML system is compatible with outputs from the WRF meso-scale meteorological model and the CMAQ, CAMx and EMEP4UK regional air quality models. The RML system has been designed to be extendable to other regional models. Please contact CERC if there is another regional air quality or meteorological model which you would like to use.

1.2 ADMS-Urban RML system features

The principal features of the ADMS-Urban RML system are:

- A user-friendly graphical interface;
- An automated control system with logging of progress to file and screen;
- Integration with CERC's Run Manager software (CERC, 2014b) for distributing ADMS-Urban runs across multiple machines;
- Compatibility with the widely-used regional air pollution models CMAQ and CAMx;
- Flexibility regarding the size and shape of the nesting domain;
- No requirement to re-run the regional air quality or meteorological models;
- Automatic division of a large nesting domain into separate runs for each regional model grid cell, with appropriate local meteorology from the WRF meso-scale model and background concentrations;
- Inclusion of advanced modelling techniques for urban areas through the use of ADMS-Urban, such as street canyon and urban canopy flowfield calculations; and
- Output files in portable netCDF format with a utility to extract statistics such as percentiles to ADMS-format text files, which can then be used in the standard ADMS-Urban contour plotting utilities and the MyAir Model Evaluation Toolkit (Stidworthy *et al.*, 2013).

1.3 Overview of the ADMS-Urban RML system

The ADMS-Urban RML system uses output meteorological and concentration data from regional modelling to provide inputs to ADMS-Urban model runs, and calculates nested output concentrations from a combination of the regional and ADMS-Urban output concentrations.

1.3.1 ADMS-Urban RML system components

The main components of the RML system are as follows:

- the ADMS-Urban local dispersion model (McHugh *et al.*, 1997);
- the Run Manager software for distributing ADMS-Urban runs across multiple machines (CERC, 2014b); and
- the ADMS-Urban RML Controller, which consists of a graphical user interface, control program and five utility programs.

The ADMS-Urban RML system license covers the ADMS-Urban RML Controller, while separate licences are required for ADMS-Urban and Run Manager.

The main inputs to the RML system are:

meteorological data output files from the WRF meso-scale model;

- concentration data output files from the CMAQ, CAMx or EMEP4UK regional models;
- three ADMS-Urban model parameter files (.upl) containing local emissions data and definitions of output locations and species; and
- ADMS-Urban RML system parameters saved in an .npl file, created from the ADMS-Urban RML Controller interface.

The regional meteorological and concentration data can be created by the user of the ADMS-Urban RML system or obtained from a third party.

1.3.2 User methodology

The tasks which the user must carry out for a complete run of the ADMS-Urban RML system are as follows:

- **Step 1** Set up and run the WRF meso-scale meteorological model;
- **Step 2** Compile an emissions inventory appropriate for use in both local and regional dispersion modelling, including both gridded and explicit source data;
- **Step 3** Set up and run a regional dispersion model such as CMAQ, CAMx or EMEP4UK;
- **Step 4** Set up three ADMS-Urban model input (.*upl*) files:
 - A .upl file containing emissions equivalent to those used in the regional model;
 - A .upl file containing the highest available resolution emissions data for the modelling area, including explicit definitions of road and point sources; and
 - A .upl file containing the gridded equivalent of the emissions in the .upl above;
- **Step 5** Set up an ADMS-Urban RML system input (.npl) file for validation at monitor locations; run the ADMS-Urban RML system initially using the verification option to check the validity of inputs and then in full; and
- **Step 6** Set up and run an ADMS-Urban RML system input (.npl) file for contours of concentration (air quality maps).

Guidance for setting up the ADMS-Urban RML system input files can be found in Section 4 Details of how to set up each of the three ADMS-Urban input files are given in Section 4.4.1.

Instructions for installing and configuring the components of the ADMS-Urban RML system, which should be carried out before setting up the ADMS-Urban input files, are given in Section 2.2.

Note that if the regional model output data are obtained from a third party, information about the regional model emissions and some other inputs must also be obtained, as described in Section 3.

1.4 Overview of the ADMS-Urban RML User Guide

This *ADMS-Urban RML User Guide* is both a manual and a technical summary of the RML system. The contents are discussed briefly below.

Familiarity with ADMS-Urban is assumed throughout this user guide, please refer to the ADMS-Urban User Guide (CERC, 2014a) for details of standard ADMS-Urban installation, inputs and runs. Similarly, details of standard Run Manager installation and configuration can be found in the Run Manager User Guide (CERC, 2014b). Training in the use of ADMS-Urban and the ADMS-Urban RML system is available from CERC.

Section 2 describes the computational resource requirements for running the ADMS-Urban RML system, gives instructions for installing the ADMS-Urban RML system, including configuration instructions for both Run Manager and the RML Controller. It also describes the keyboard shortcuts and menu options available in the RML Controller interface.

Running the ADMS-Urban RML system requires various sources of data in addition to those needed for a stand-alone ADMS-Urban run. The additional requirements, in particular those relating to consistency with the chosen regional model, are described in Section 3.

Each screen of the RML Controller interface and all the user options are covered in Section 4. This section also includes details of how to set up the three ADMS-Urban .upl input files used in the ADMS-Urban RML system.

Section 5 describes the output files from the ADMS-Urban RML system and methods for processing the concentration outputs from the RML system.

Some guidance on how to investigate and solve common errors is given in Section 6

Three worked examples showing how to use the ADMS-Urban RML system to obtain concentrations at receptor locations or for contours are given in Section 7. The files required to run these worked examples are supplied as part of the ADMS-Urban RML Controller installation.

A technical summary of the concept and implementation of the RML system is given in Section 8. Each procedure required to generate nesting output concentrations for receptor and gridded output locations is described. Features of ADMS-Urban and Run Manager which are not used in their stand-alone applications are also described, along with the limits of the RML system.

References are given in Section 9.

Each of the utility programs used in the RML system are described in an appendix. Appendix A gives details of the utility used to extract ADMS-format meteorological data from WRF. The utility for extracting background concentrations from the regional air quality model files is described in Appendix B. Appendix C concerns the utility for calculating nesting output concentrations and Appendix D the utility for re-combining results from multiple spatial domains. The final utility in the RML system, used for adding interpolated source-oriented grid points to output files, is described in Appendix E.

1.5 Conventions

To make this user guide simpler to use, certain conventions have been followed with regard to layout and style.

- ADMS-Urban RML Controller interface controls are shown in **Arial** font, e.g. the **Grids** screen, click on the **Plot** button.
- Keyboard keys are shown in **bold**, e.g. press **Enter**.
- Directory and file names are shown in *italics*, e.g. *WRFtoMet.exe*, <*install_path*>*Data*.
- Tips and other notes are shown thus:

Think about the area you want to include in the calculation before specifying the output grid.

• Table and figure references are shown in **bold**, e.g. refer to **Table 3.2**, **Figure 2.1**.

SECTION 2 Getting started

2.1 System requirements

It is possible to run the ADMS-Urban RML system on a single PC, however it is more efficient to divide the RML system across at least two PCs, as depicted in **Figure 2.1** and described below.

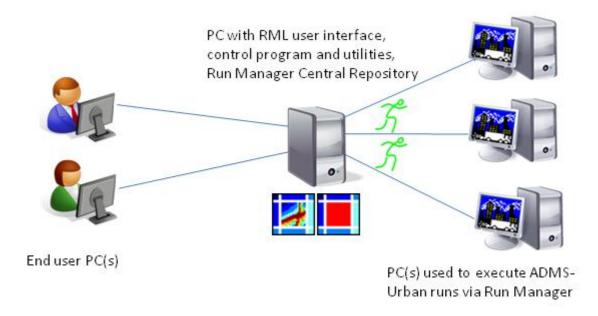


Figure 2.1 Schematic of the RML system installation with one PC used for the RML Controller user interface, control program and utilities, and one or more used for ADMS-Urban runs.

One machine has the ADMS-Urban RML Controller installed, so the user can set up ADMS-Urban RML system parameter files (.npl); the ADMS-Urban RML Controller will run on this machine. This machine must also have Run Manager installed and configured so that the RML Controller can submit ADMS-Urban runs via Run Manager. It may be convenient to locate the Run Manager central repository on this machine.

All other PCs have Run Manager and ADMS-Urban installed and are used to carry out the ADMS-Urban model runs. If multiple processors and sufficient RAM are available on these PCs, and sufficient ADMS-Urban licenses are available, multiple simultaneous ADMS-Urban runs can performed on each machine, which will improve overall run times for the RML system, particularly for a large nesting domain.

Note that multiple instances of the ADMS-Urban RML Controller cannot be run simultaneously using the same controller machine. If you wish to run multiple ADMS-Urban RML system configurations, these should be set up to run sequentially with the same controller machine, or simultaneously on different controller machines, if you have a multiuser licence for the ADMS-Urban RML system.

The operating systems on which each major component of the ADMS-Urban RML is currently supported are listed in **Table 2.1**.

Please contact CERC if you would like to run ADMS-Urban on a Linux system via Run Manager.

Program	Version used in ADMS-Urban RML system	Supported operating systems
ADMS-Urban RML Controller	1.1	Windows 7, 8.1
Run Manager	1.5	Windows 7, 8.1
ADMS-Urban model	3.4	Windows 7, 8.1

Table 2.1 List of software components of the ADMS-Urban RML system with current version numbers and supported operating systems.

The working memory (RAM) and disk space required for an ADMS-Urban RML system run will vary according to the chosen inputs. Specifically, the number of regional model grid cells included in the nesting domain, the number of sources in each ADMS-Urban model parameter file (.upl) and the number of modelled hours can all affect the disk space required for an ADMS-Urban RML system run.

The worked examples supplied with the ADMS-Urban RML system include files for three runs of a 2 x 3 cell nesting domain for 72 model hours, with different numbers of output points and file save options. The files from these runs occupy approximately 200 MB of disk space. However a large, high resolution contour run (15 x 17 cells) for a full year may require tens of GB of disk space. Hence the disk space requirements for the ADMS-Urban working directory and .npl directories will depend on the spatial and temporal extents of the modelling.

2.2 Installing the ADMS-Urban RML system

The ADMS-Urban RML system requires ADMS-Urban and Run Manager to be installed and configured in order to run correctly. Please refer to the ADMS-Urban User Guide for general information about installing the ADMS-Urban model software, and the Run Manager User Guide for general information about installing Run Manager. These User Guides are available from the *Documents* sub-directory of the relevant installation directory, or from the CERC website. Some specific information and advice about how to configure Run Manager for use by the ADMS-Urban RML Controller is given in Section 2.2.1.

The installation of the ADMS-Urban RML Controller is straightforward. It uses an Installation Wizard, which guides the user through a short series of screens, obtaining information about user preferences and installation parameters, before installing the software. The installation process for the ADMS-Urban RML Controller is described in detail in Section 2.2.2. After installation, the user must set some local configuration parameters as described in Section 2.2.3.

Please check your company procedures for installing software with your local IT personnel before installing the ADMS-Urban RML system.

2.2.1 Installing and configuring Run Manager

Please follow the installation instructions in the Run Manager User Guide (CERC, 2014b) to install Run Manager on the RML Controller machine and any runs machines. Set up a central repository directory and link all the machines to it, as described in the Initial Configuration section of the Run Manager User Guide. Ensure that all machines using Run Manager can read from and write to the central repository directory.

Set an appropriate Run Manager working directory and maximum number of concurrent runs for any runs machines, as described in the Defining Local Settings section of the Run Manager User Guide.

Set up an ADMS-Urban model and an execution group for use by the ADMS-Urban RML Controller, following the instructions in the Defining Models and Defining Execution Groups sections of the Run Manager User Guide.

It is advisable to set up a dedicated Run Manager model and execution group for ADMS-Urban runs within the ADMS-Urban RML system, to ensure that they can be identified, particularly if your Run Manager installation and runs machines will also be used for stand-alone ADMS-Urban runs.

2.2.2 Installing the ADMS-Urban RML Controller

The following steps lead you through the ADMS-Urban RML Controller installation process.

- **Step 1** Log on as Local Administrator for the PC.
- **Step 2** ADMS-Urban RML Controller will either have been supplied by download link or on CD. Follow the appropriate instructions:

Download: Unzip the downloaded .zip file to a local directory. In Explorer, browse to this directory and double-click on the file 'setup.exe'.

CD: Insert the installation CD and the install program should automatically start. If it does not, browse to locate the CD in Explorer and double-click on the file 'setup.exe'.

In both cases, the screen shown in **Figure 2.2** will be launched.

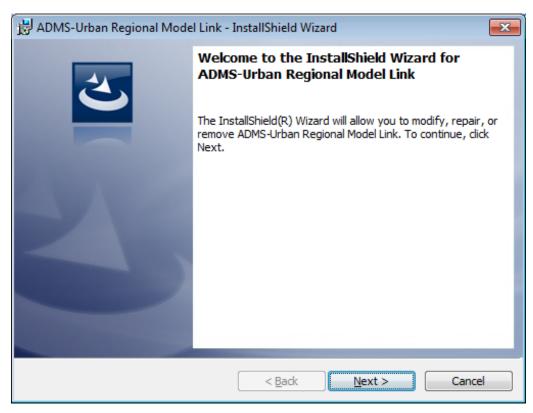


Figure 2.2 – The ADMS-Urban RML Controller installation welcome screen.

Step 3 Click Next > through the welcome screen. The Customer Information screen is then displayed, as shown in Figure 2.3.

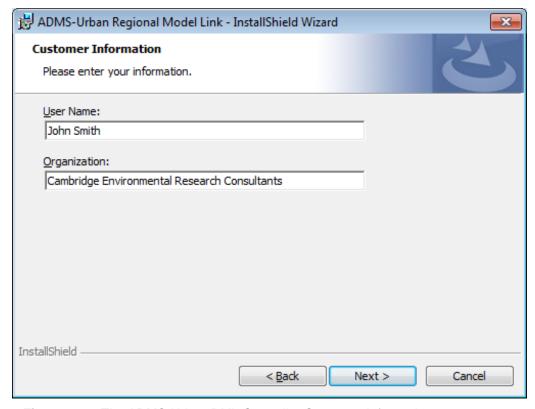


Figure 2.3 – The ADMS-Urban RML Controller Customer Information screen.

Step 4 Enter your user name and organisation in the designated places. Click Next > to go through to the Destination Folder screen, as shown in Figure 2.4.

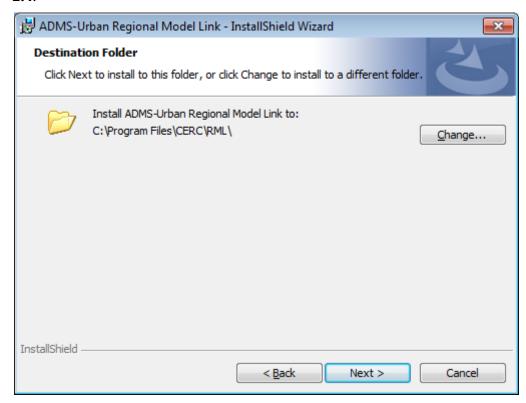


Figure 2.4 - The ADMS-Urban RML Controller Destination Folder screen.

Step 5 You should select a drive with at least 1 GB of available disk space.

Note that the user will need read and write permissions for both the *.ini file (in the installation directory) and the working directory of the ADMS-Urban RML Controller.

The default installation directory is $C:\Program\ Files\CERC\RML$ on a 32-bit Windows system, or $C:\Program\ Files\ (x86)\CERC\RML$ on a 64-bit machine. If required, use the **Change**... button to select your own installation directory (**Figure 2.5**). Click **OK** to return to the Destination Folder screen.

The abbreviation <install_path> will be used in the rest of the User Guide to denote the installation directory you have chosen, for example C:\Program Files\CERC\RML.

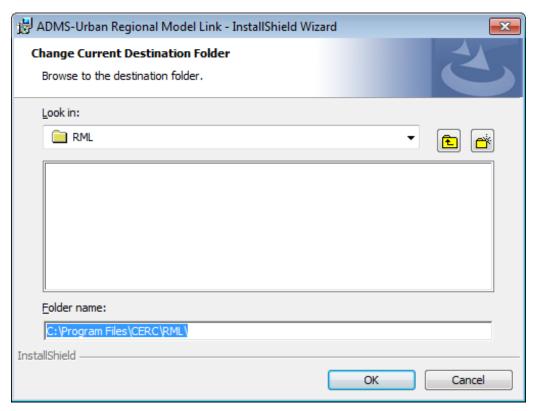


Figure 2.5 – The Change Current Destination Folder screen.

Click **Next>** to choose who should be able to use the ADMS-Urban RML Controller, as shown in **Figure 2.6**.

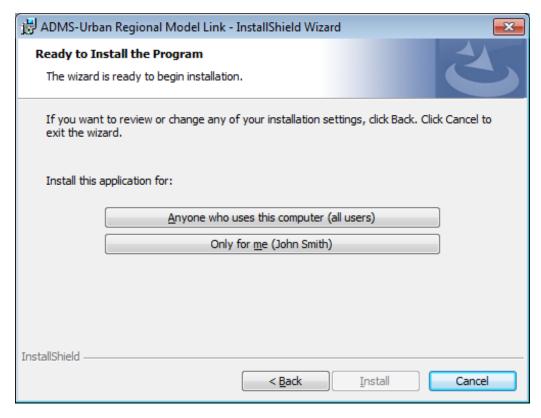


Figure 2.6 - The Ready to Install the Program screen.

Step 6 Choose whether to install for all users or just the current user.

If the user profile being used for installation (for example, a local administrator profile) is not the usual user profile, choose to install for all users.

If you first wish to amend any details, press the **< Back** and **Next >** buttons as appropriate. Once the **Install** button has been pressed, and the ADMS-Urban RML Controller files have been successfully installed, the final screen will appear, as shown in **Figure 2.7**.

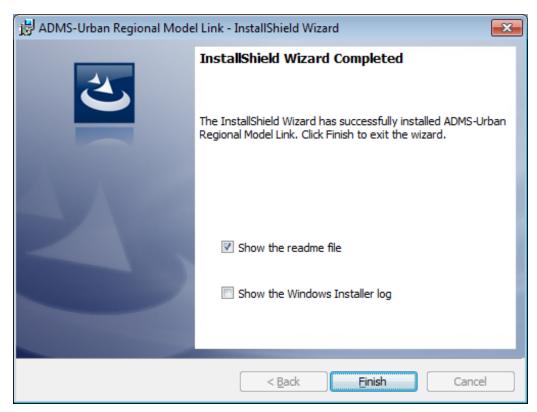


Figure 2.7 – The ADMS-Urban RML Controller Installation Wizard Completed screen.

Step 7 Click Finish to complete the installation. The installation procedure automatically adds a shortcut to ADMS-Urban RML Controller on your Windows desktop. If the Show the readme file box is checked the document ADMS-Urban RML User Guide.pdf will be opened automatically once you click on Finish. If the Show the Windows Installer log is checked then the install log will be opened automatically once you click on Finish.

The installation is now complete.

You have been provided with a unique licence file, by email, which is required in order to run the model. It is important that you install this new licence file as instructed.

Step 8 To install the ADMS-Urban RML Controller licence, rename the emailed file to *RML-Cont.lic* and copy it to the *<install_path>* directory.

Step 9 Restart your computer: you are now ready to use the RML system.

2.2.3 Configuring the ADMS-Urban RML Controller

The ADMS-Urban RML Controller needs to be able to access the Run Manager central repository directory in order to send ADMS-Urban runs to Run Manager. Identify the location of the Run Manager central repository by selecting the File\Change Run Manager Repository menu option and browsing to the central repository directory.

Some optional configuration settings can be defined in the .ini file for the ADMS-Urban RML Controller, which can be found as <install_path>\RML-Controller.ini.

Open the .ini file in a text editor, such as Notepad, make the required changes and save the file. The default RML-Controller.ini file is shown in **Figure 2.8**.

If you wish to change any settings in the .ini file, it is advisable first to save a back-up copy of the original file.

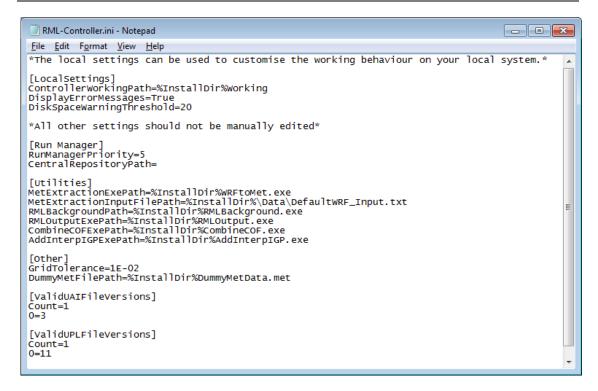


Figure 2.8 The default RML-Controller.ini file opened in Notepad for editing

There are three parameters which may be set by the user in the ADMS-Urban RML Controller .ini file:

• ControllerWorkingPath — this is the location of the ADMS-Urban RML Controller working directory, by default <install_path>\Working. Careful consideration of the location of the ADMS-Urban RML Controller working directory is strongly recommended. The working directory is used by the ADMS-Urban RML Controller to store input, intermediate and output files during each run, depending on the choice of Output type. All user profile(s) that will run the ADMS-Urban RML Controller will require read, write and modify permissions for the working directory. Note also that the majority of

the disk space required by the RML Controller is used by the working directory.

- DisplayErrorMessages whether error messages from the RML Controller should be displayed as pop-up windows (True, by default) or just written to the log file (False), for example for automated runs; and
- DiskSpaceWarningThreshold the threshold of disk space (in GB) available in the ADMS-Urban RML Controller working directory, below which a warning should be issued, by default 20 GB.

It is recommended to use a local directory (eg. D:\) or mapped network drive (eg. Z:\), not an external drive (eg. \\Computername\dir\), as the working directory for the ADMS-Urban RML Controller, to allow the RML Controller to check the available disk space. Ensure the RML Controller working directory has appropriate permissions set.

Note that the working directory may require a large disk space if large runs are being performed by the ADMS-Urban RML system, and the system will fail if insufficient disk space is available.

2.3 Introduction to the ADMS-Urban RML Controller interface

This section gives an overview of the functions of the ADMS-Urban RML Controller interface. For more information about each component of the interface, with advice on suitable inputs and settings, please refer to Section 2.4 for menu items and Section 4 for modelling scenario parameters.

2.3.1 Mouse buttons

Unless otherwise stated, mouse instructions refer to the left button. If the mouse options have been used to reverse the mapping (e.g. because you are left-handed), the right mouse button should be used instead.

2.3.2 Keyboard access

All mouse instructions in this User Guide can be reproduced using keystrokes. A brief guide to these keystrokes is given in **Table 2.2**.

Also known as shortcut keys, there are combinations of keys that perform some of the main commands. For example, menu commands that have one letter underlined are accessible by holding down the ALT key and then typing the underlined letter. For example, the menu command \underline{Open} ... located on the \underline{File} menu, may be executed by typing ALT + F and then ALT + O.

Key	Description		
Moving the cursor between data entry boxes			
TAB	Move the cursor forward through data entry boxes or buttons		
SHIFT + TAB	IFT + TAB Move the cursor backwards through data entry boxes and buttons		
RETURN 'Enter' or accept the current data page or execute the action of highlighted button			
SPACEBAR	CEBAR Select or deselect the highlighted option		

Entering data in a box

DELETE	Delete the character immediately to the right of the cursor		
BACKSPACE	ACE Delete the character immediately to the left of the cursor		
← arrow	Move the cursor one space to the left in the current box		
→ arrow	Move the cursor one space to the right in the current box		
SHIFT + Begin highlighting characters in the direction of the arrow (see			
arrow	above)		

Highlighted text

DELETE	Delete all highlighted characters
(Type)	Typing text replaces the highlighted text with new text

Table 2.2 Keystrokes to enable you to move through the ADMS-Urban RML Controller interface.

2.4 Menu options

The menu bar has five headings: File, Run, Results, Utilities, and Help. Clicking on any of the headings leads to a drop-down list of options, as shown in Figure 2.9 for the File heading. Table 2.3 lists all the available options with references to further details of their use.

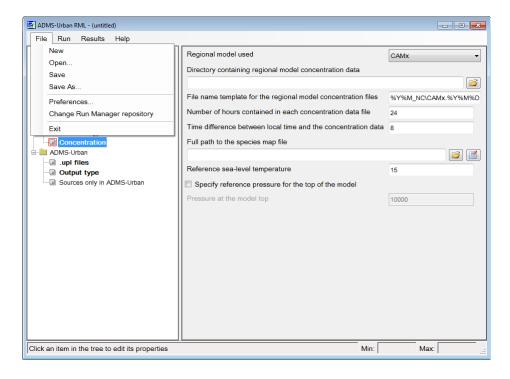


Figure 2.9 The File menu from the menu bar in the ADMS-Urban RML Controller interface.

Menu	Item	Description	Reference
		Reset the parameters in	
	New	the .npl file to their	
		default values	
		Allow the user to open a	
	Open	previously saved	
		parameter file	
		Save the current	
	Save	parameters under the	
File		current file name	
		Save the current	
	Save As	parameters with a user-	
		specified file name	
	Preferences	Set interface preferences	2.4.1
	Change Run Manager Repository	Select the location of the	2.2.3
		Run Manager repository	
	Exit	Quit ADMS-Urban RML	
		Controller interface	
		Run the RML system	
	Model	using the current	2.5.4
		parameters	
		Run the RML system	
Run		using the current	
Kuli		parameters for a small	
	Model verification	number of hours to	2.5.4
		verify inputs and	
		check disk space	
		requirements	
		Launch the ADMS	
		Comprehensive Output	
	Future of Chatlatian	File Processor with the	щ.
	Extract Statistics	output file from the .npl	#
Results		currently loaded in the	
		interface	
		Open the log file for the	
	View log file	latest run in the preferred	5.1.1, 2.4.1
		viewing program	
	User Guide	Open the User Guide in	
	Oct Ouide	the default pdf viewer	
		Auto-address a new	
	Email CERC	email to the CERC	
Help		helpdesk in the user's	
۲.۰۰۳		default email client	
		Show RML system and	
1	About ADMS-Urban RML	RML Controller	
ĺ	o o i wait talle	interface version	
	2 List of many itams with describe	numbers	

Table 2.3 List of menu items with descriptions. The last column (Reference) indicates the section of the user guide where the item is further described, where appropriate. #Please refer to the *ADMS Comprehensive Output File Processor User Guide* (CERC, 2014c) for more details.

2.4.1 Setting ADMS-Urban RML Controller interface preferences

Two preferences for the behaviour of the RML Controller interface can be defined using the File\Preferences... menu option. The Preferences screen is shown in Figure 2.10.

On the **Viewing** tab, shown in **Figure 2.10**, the default application for viewing input text or comma-separated variable files and the ADMS-Urban RML Controller log file can be chosen. If you wish to use an application other than the three default choices given on the screen, choose the **Other** option and type or paste the file-path to the application executable (*.exe*), with any required command-line arguments, into the box.

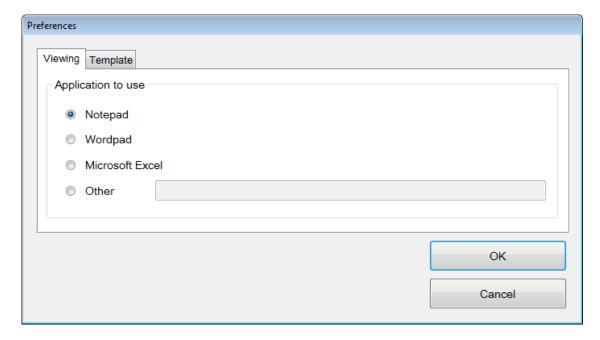


Figure 2.10 The Viewing tab of the Preferences dialogue

A template data file may be chosen using the **Template** tab, shown in **Figure 2.11**. This data file is an *.npl* file, which may be complete or incomplete, with the default settings you would like to be included every time you create a new *.npl* scenario file. For example, this default file may be used to define your Run Manager model name and execution group name. To create a template *.npl* file, use the RML Controller interface to set the options you would like and save the *.npl*. Then choose the **Use a template data file** option on the **Template** tab of the **Preferences** screen and use the **Browse** button (\square) to select the template *.npl* file. Click **OK** to save your preferences.

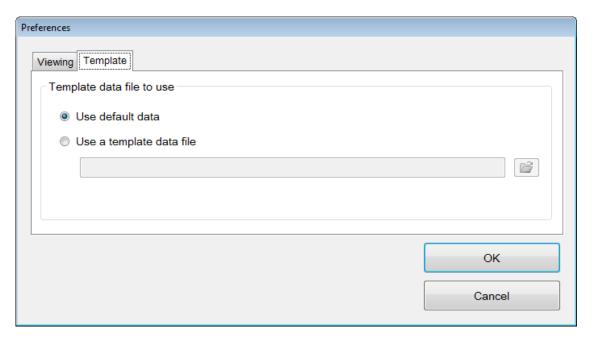


Figure 2.11 The Template tab of the Preferences dialogue

2.5 Creating a control file and running the ADMS-Urban RML system

Section 1.3.2 describes the full user methodology for modelling using the ADMS-Urban RML system. If the regional model data are already available and all components of the system are correctly installed and configured, the following steps must be taken to generate results from the RML system:

- create a new ADMS-Urban RML system parameters file (.npl),
- enter data to define the problem,
- save the ADMS-Urban RML system parameters file,
- run the ADMS-Urban RML system and
- display the output generated by the ADMS-Urban RML system.

The first four of these steps are described in Sections 2.5.1 to 2.5.4. Entering model data is described in general terms here, and in full detail in Section 4. Displaying model output is covered in Section 5.

2.5.1 Creating a model file

When the ADMS-Urban RML Controller interface is loaded or when you select the **New** command from the **File** menu, a new model file, or scenario, is created and default values are loaded into the screens for you to edit.

To open an existing model file for editing or execution, choose **Open**... from the **File** menu. By default, the RML Controller interface will display only files with the .npl extension.

2.5.2 Entering information

RML Controller Interface layout

The interface window has two main panels: on the left hand side a tree structure of sections and screens is displayed, while on the right hand side the entries for the current screen are displayed. The icon for the current screen is indicated with a red outline in the tree structure panel, as shown in **Figure 2.12**. A particular screen can be viewed or edited by clicking on it in the tree structure.

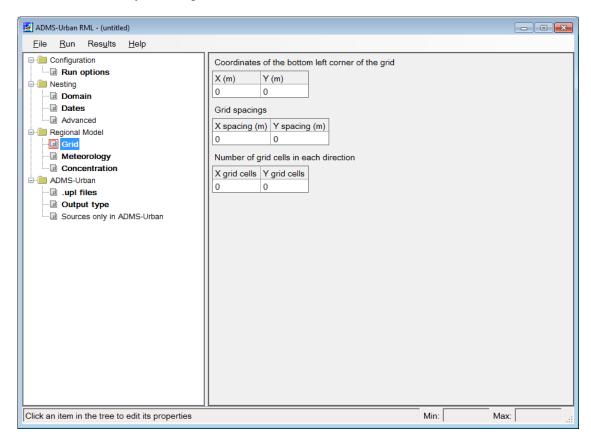


Figure 2.12 The ADMS-Urban RML Controller interface with the **Grid** screen of the **Regional Model** section selected for editing

Changing values in the input screens

To change a parameter value in an input screen, move the pointer until it is over the appropriate text box and click. Alternatively, use the **TAB** or **arrow keys** to move systematically through the sections contained in each screen. The selected area will be highlighted. Typing a new value will automatically replace what was highlighted. Alternatively, use **DELETE** and/or **BACKSPACE** to remove unwanted characters before typing in the new value.

Note that a blank cell does not denote a value of zero.

The helpline

This is a single line of text that appears at the bottom of the active screen. The information in the helpline changes when different items are selected on the screen.

The helpline gives a brief description of the selected control's function. Where you are prompted for a numerical value, the helpline will give the units and the maximum and minimum values allowed.

For example, when you click in the box to set the reference sea-level temperature, the helpline will display the following:

Reference sea-level temperature, used for converting vertical level coordinate values into heights (°C) Min: -50 Max: 50

Data validity and integrity checking

As you enter data, the ADMS-Urban RML Controller interface performs checks to ensure that all user-entered data are consistent with the model's logic and that maximum and minimum values are satisfied.

2.5.3 Saving input data to a parameter file

When you are ready to run the ADMS-Urban RML system, choose **Save** from the **File** menu of the RML Controller interface. If the current scenario has not been saved before, you will be prompted to choose a directory and file name. ADMS-Urban RML Controller files are always saved with the extension .npl. The results and output files of the ADMS-Urban RML system run will be saved to the directory in which the .npl file is saved.

2.5.4 Running the ADMS-Urban RML system

Having saved the current scenario as an .npl file, go to the menu bar and click on Run then Model to run the ADMS-Urban RML system. If the current scenario has not yet been saved or if you have changed anything in the RML Controller interface since the scenario was last saved, then you will be prompted to save the modifications.

When setting up a large run of the ADMS-Urban RML system, it is recommended to test the system inputs by initially running in verification mode, which runs the system for a small number of hours. This will allow you to verify your inputs and to estimate the disk space required to store the complete run. To run the system in verification mode with the currently loaded .npl file, select Run then Model verification.

Note that neither the duration nor the disk space requirement of the complete run is linearly related to the duration of the verification run, due to overheads of initial processing task time and file structure, however an upper estimate for the disk space required for the complete run will be proportional to the increase in the number of modelled hours when compared to the verification run.

Alternatively, you can run the RML system using a batch file. These files allow you to run several files consecutively without opening and running each .npl separately, or to schedule runs of the ADMS-Urban RML as part of an automated system. Please refer to Section 2.6 for details of the batch file format for running the ADMS-Urban RML system.

While the RML system is running, the status of the various tasks performed by the system is reported via a progress window (as shown in **Figure 2.13**). When all the calculations have successfully completed, the progress window displays "RML system run completed" and a notification window appears, as shown in **Figure 2.14**.

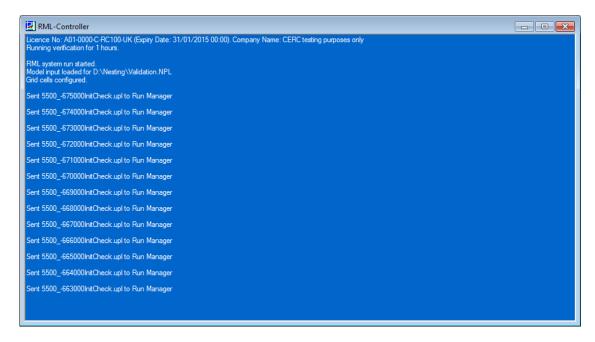


Figure 2.13 Progress window of an ADMS-Urban RML system run

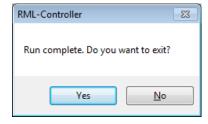


Figure 2.14 Completion notification window of an ADMS-Urban RML system run

The progress of the ADMS-Urban runs used in the RML system can be monitored using the Run Manager Run Status screen, as shown in Figure 2.15. RML system ADMS-Urban runs should not be modified manually in Run Manager unless there has been a failure on the controlling or run machines.

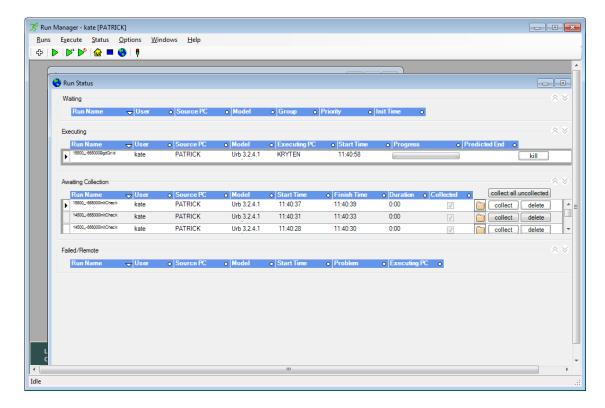


Figure 2.15 Run Manager Run Status screen showing ADMS-Urban runs from the ADMS-Urban RML system

Runtime preferences

The user can edit runtime options for the ADMS-Urban RML system in the **Configuration**, **Run options** section of the RML Controller interface. Please refer to Section 2.2.3 for more details of the available options.

Cancelling a run

It is possible to cancel an ADMS-Urban RML system run which is in progress, for example in order to alter an input parameter, by closing the progress window (as shown in **Figure 2.13**).

In rare circumstances ADMS-Urban runs in progress may leave files on the run machine, which can be deleted via Run Manager. If the runs machine or nesting controller machine fail during a run, some manual file deletion may also be required. Please refer to Section 6.5.1 for more details of how to identify and delete failed or unwanted runs in Run Manager.

2.5.5 Displaying model output

Please refer to Section 5.2 for details about displaying or otherwise processing output from ADMS-Urban RML system runs.

2.6 Running the ADMS-Urban RML system automatically

The ADMS-Urban RML system can be run automatically, for example as part of a forecasting system or to allow a series of runs with different parameters, using batch files. A batch file is a plain text file with .bat extension, which contains DOS commands. The contents of a batch file are not case-sensitive.

The batch file syntax for a typical ADMS-Urban RML system run is:

```
<RML controller path name> /e2 <.ini path name> <.npl file path name>
```

where:

- <RML controller path name> is the full path name of the ADMS-Urban RML Controller executable file (*RML-Controller.exe*, located in the ADMS-Urban RML Controller installation directory), enclosed in inverted commas (");
- /e2 is an option to cancel the prompt window at the end of the system run;
- <.ini path name> is the full path name of the ADMS-Urban RML Controller interface configuration file (*QUAD.ini*, by default located in the ADMS-Urban RML Controller installation directory), enclosed in inverted commas ("); and
- <.npl file path name> is the full path name of the .npl file you wish to run, enclosed in inverted commas (").

For example, if the ADMS-Urban RML Controller is installed in the default installation directory ($C:\Program\ Files\ (x86)\CERC\Regional\ Model\ Link$) and the .npl file to run is $D:\My\ Work\Test.npl$, the contents of the batch file could be:

```
set InstallDir = C:\Program Files (x86)\CERC\Regional Model Link
"%InstallDir%\RML-Controller.exe" /e2 "%InstallDir%\QUAD.ini" "D:\My
Work\Test.npl"
```

The second command can be repeated for each *.npl* you would like to run. Any additional run mode options which you would like to specify, for example /verify for a model verification run, should be inserted before the *.ini* file path name. To start the ADMS-Urban RML system run, double click on the *.bat* file in Windows Explorer.

Note that for automatic runs of the ADMS-Urban RML system, the RML Controller configuration option to switch off error message boxes should be selected. Please refer to Section 2.2.3 for more information about ADMS-Urban RML Controller configuration options.

SECTION 3 Data requirements

The ADMS-Urban model User Guide describes the general input data required to run the ADMS-Urban model for stand-alone simulations, typically using measured meteorology and background concentrations. Additional requirements for the ADMS-Urban RML system are described in this section, with specific information about meteorology, emissions, regional model output concentrations and other requirements. It is important for the validity of the final nested concentration output that consistent data is used for the different components of the modelling system, in particular for the time-variation of gridded emissions.

If you are obtaining regional model output data from a third-party provider, please note that related information about the regional model inputs is also required.

3.1 Coordinate system

All spatially-varying inputs to ADMS-Urban must be defined in the same projected coordinate system with units of metres. This coordinate system should be consistent with the regional model grid definition, so that the regional model grid is rectilinear in the chosen coordinate system. The WRF model coordinate system is required to use either the Lambert Conformal Conic or Polar Stereographic projection with no false easting or false northing.

Note that the regional model horizontal grid must be regular but is not required to be isotropic (equal spacing in x and y directions).

The vertical grid definition for the regional meteorological and concentration outputs must use sigma (pressure) coordinates.

3.2 Meteorology

The ADMS-Urban RML system extracts meteorological data from the meso-scale model WRF. Each model grid cell which is included in the nesting domain uses meteorology from the corresponding WRF grid cell.

The WRF data used in the ADMS-Urban RML system should be the same as that used to run the regional photochemical model, with a consistent grid definition. Each WRF output file should contain exactly one hour of data, with at least the following variables:

- Wind speed components in the x and y directions (U and V), either at 10 m or at each vertical grid level in the latter case, height variables must also be available; and
- Incoming solar radiation or surface sensible heat flux.

Other variables which can be extracted for use as input to the ADMS-Urban run include boundary layer height and precipitation. The most suitable combination of variables may depend on the meteorological pre-processor used for the regional model.

A value of roughness length consistent with that used by WRF within the nesting domain should be entered into the ADMS-Urban interface. WRF output files may contain values of roughness length or dominant land use category values which are each associated with a value of roughness length. The roughness length chosen for use in ADMS-Urban should reflect the value used by WRF for the areas with highest emissions within the nesting domain. For the main ADMS-Urban runs in the RML system, the integrated urban canopy flow field module can be used to calculate local values of roughness based on building parameters, which may be more appropriate for local modelling than the dominant land use values in WRF.

The WRF output file names must be compatible with use on a Windows operating system — note that the default output file names include ':' characters in the date part of the file name which are not compatible with Windows. The file paths and names should follow a pattern which indicates the date and time of the data contained within the file.

For full details of the utility which is used to extract ADMS format met data from WRF output files in the ADMS-Urban RML system, which can also be used as a stand-alone program, please refer to Appendix A.

3.3 Emissions

In addition to the standard emissions data which is required to model an urban area using ADMS-Urban, for the ADMS-Urban RML system, gridded emissions data consistent with that used in the regional model must be processed in order to obtain valid nesting background concentrations, as described in Section 4.4. Both the total emissions and the time-variation of emissions should be matched as closely as possible to the regional model equivalents. The ADMS-Urban grid source resolution and grid cell horizontal geometry should correspond to that in the relevant regional model domain. The grid source depth defined in ADMS-Urban should be set to twice the depth of the regional model grid layer(s) containing the majority of ground-level emissions. Please refer to Section 4.4.1.1 for more details of the ADMS-Urban inputs for this run.

3.4 Regional model concentrations

Regional air quality models usually contain more detailed chemistry schemes, with a larger number of chemical species, than are required in a local model such as ADMS-Urban. For example, regional models generally use NO and NO₂ for nitrogen chemistry rather than NO₂ and NO_x, so the regional model NO_x concentration must be calculated in the RML Controller utilities by combining NO and NO₂ in order to use the ADMS-Urban NO_x chemistry module. In order for the ADMS-Urban RML system to take into account local chemistry effects, a 'species map' must be defined, which contains the factors used to convert between regional model and ADMS-Urban species and units.

It is possible to model individual particulate species in ADMS-Urban if the emissions data are defined with the same species, however it is more common to model 'lumped' particulates such as PM₁₀ and PM_{2.5}, as these are the classifications by which concentrations are most commonly measured and for which air quality standards and objectives are specified. If the ADMS-Urban sulphate chemistry module is required, in order to include local conversion of SO₂ to PM_{2.5} and PM₁₀, lumped particulate species must be used in ADMS-Urban.

Please refer to Section 4.3.3.6 for more details of the species mapping method used in the ADMS-Urban RML system.

The regional model concentration output file names must be compatible with use on a Windows operating system. The file paths and names should follow a pattern which indicates the date and time of the first valid hour of data contained within the file.

The regional model output concentration files should contain hourly average concentrations from each hour of the modelling period. Each file can contain one or more hours of data.

3.5 Other information

ADMS-Urban runs in local solar time, whereas meso-scale meteorological and air quality models often run in UTC. The user is required to specify the time difference between the regional model data and local solar time.

SECTION 4 System inputs

Before running the ADMS-Urban RML system, the user needs to define the system inputs, for example the file locations of regional model outputs. This section provides a guide to the ADMS-Urban RML Controller interface with discussion of the available options. The opening screen of the RML Controller interface is shown in **Figure 4.1**. Individual sections of the interface can be selected from the tree structure on the left, while data and modelling options are entered on the right.

Data must be entered into at least eight screens to specify configuration options, the spatial and temporal extents of the modelling domain, the regional model output format, the ADMS-Urban model input files and the required output type. It is advisable, though not necessary, to work through each section of the RML Controller interface in turn, starting at the top of the tree structure.

Note that incomplete .npl *files can be saved for later completion, or for use as templates.*

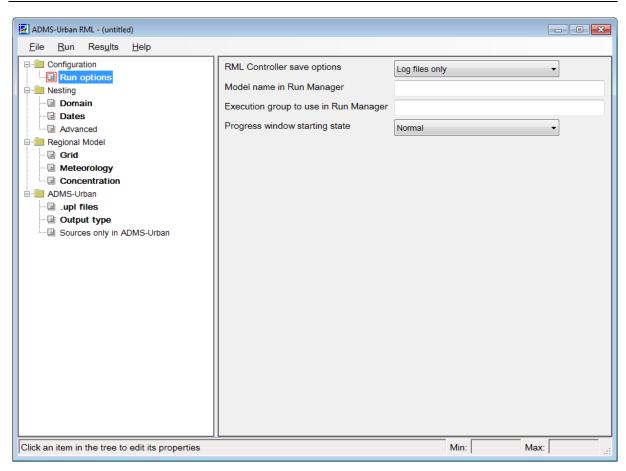


Figure 4.1 The ADMS-Urban RML Controller interface

4.1 Configuration

The **Configuration** section of the ADMS-Urban RML Controller interface contains options which may vary between runs of the ADMS-Urban RML system. Other configuration options which are unlikely to be altered frequently, such as the location of the RML Controller working directory, can be set in the *.ini* file, details of which can be found in Section 2.2.3.

4.1.1 Run options

The **Run options** screen is shown in **Figure 4.2**. This is the screen which appears when the ADMS-Urban RML Controller interface is opened. General configuration information about the behaviour of the RML Controller is entered on this screen. Each item is discussed in turn in Sections 4.1.1.1 to 4.1.1.4.

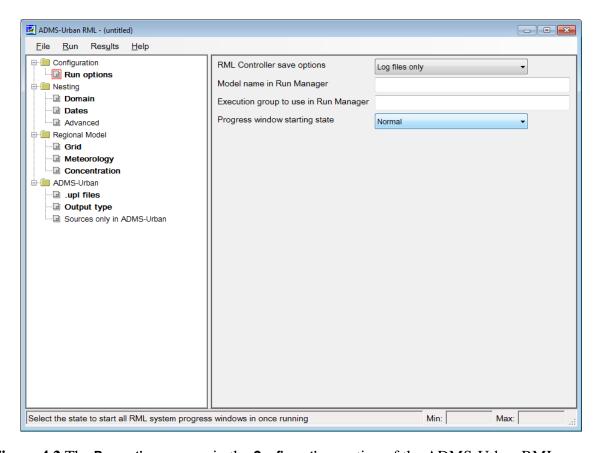


Figure 4.2 The **Run options** screen in the **Configuration** section of the ADMS-Urban RML Controller interface

4.1.1.1 RML Controller save options

The **RML Controller save options** list gives three options for the number and types of intermediate files which should be saved and returned by the ADMS-Urban RML system, in addition to the results files:

• The default option is only to keep log files, which will include any information, warning and/or error messages issued by each component of the RML system. This requires the least storage space and is suitable for all types of system runs.

• The intermediate option is to keep 'key files', which includes all ADMS-Urban format meteorology and background concentration files; these files may be useful for model validation and comparison purposes. A list of the files included in the 'key files' category is given in **Table 4.1**. If any component of the RML system fails, the input and any output files for that component will also be saved.

Note that if the nesting domain is large and the RML system is run for an extended modelling period, this option may generate a large volume of data.

• The final option is to keep all the files used in every component of the RML system, which may be useful for detailed investigation of the system behaviour. Due to the number and size of files involved in the ADMS-Urban RML system, this option is not recommended for runs with large nesting domains or large numbers of output locations.

File extension	ADMS-Urban RML component	File description	Each cell?	Each hour of Tm?
.met	Extraction of WRF met data	ADMS format met file	Y	N
.bgd	Extraction of local upwind background	ADMS format background file	Y	N
.pst	Initial ADMS-Urban run for nesting background	ADMS format specified point output file	Y	N
.bgd	Calculation of nesting background concentrations	ADMS format background file	Y	N
.nc	Main ADMS-Urban runs (gridded and explicit emissions)	ADMS comprehensive output file format	Y	Y
.тор	ADMS-Urban run with explicit emissions	ADMS processed met data output file	Y	Y
.nc	Calculation of RML output concentrations	nested output (runs for contour output only)	Y	N
.asp	Creation of .asp file containing source-oriented grid points	ADMS additional specified point location input file (runs for contour output only)	N	N
.txt	Combination of nested output from multiple grid cells	Input text file	N	N
.nc	Combination of nested output from multiple grid cells	Combined nested output prior to addition of interpolated source-oriented grid points (runs for contour output only)	N	N

Table 4.1 List and descriptions of files kept under the 'key files' option. The 'Each cell?' and 'Each hour of Tm?' columns indicate whether files are created for each regional model grid cell covered by the nesting domain and/or each hour of a mixing time greater than 1 hour, respectively.

4.1.1.2 Model name in Run Manager

The name of the ADMS-Urban model as defined in Run Manager should be entered exactly as found in the **Model** list on the **Add Runs** screen in Run Manager when submitting a run manually. The specified model executable is used for all ADMS-Urban runs in the RML system. Note that the capitalisation of the **Model** name entered in the RML Controller interface must match that used in Run Manager.

4.1.1.3 Execution group in Run Manager

The name of the desired execution group of runs machines should be entered exactly as found in the **Execution Group** drop-down list on the **Add Runs** screen of Run Manager when submitting a run manually. The same execution group is used for all ADMS-Urban runs in the RML system and the runs will be distributed between the available machines in this group by Run Manager. Note that the capitalisation of the **Execution Group** name entered in the RML Controller interface must match that used in Run Manager.

4.1.1.4 Progress window starting state

Select whether the ADMS-Urban RML Controller progress window, which shows messages about the progress of each stage of the RML system, should initially be open or minimised. This option also controls the starting state for all RML Controller utility progress windows. The user is able to alter the state of the progress windows during the ADMS-Urban RML system run.

4.2 Nesting

The **Nesting** section of the RML Controller interface contains options to specify the spatial and temporal extents of the ADMS-Urban RML system run, and some advanced parameters which control the system's behaviour.

4.2.1 Domain

The geometry of the nesting domain, which is the spatial region within which nesting calculations will be performed, is defined in the **Domain** screen, which is shown in **Figure 4.3**. The input requirements for this screen are described in Sections 4.2.1.1 and 4.2.1.2.

Note that the nesting domain must be defined to coincide with a rectangular set of regional model grid cells, to within a tolerance of 1% of the regional model grid cell size.

The nesting domain must be fully within the regional model grid, with a border of at least one unused cell in each direction, to allow the local upwind background concentrations to be calculated using the cells bordering the nesting domain for any upwind direction.

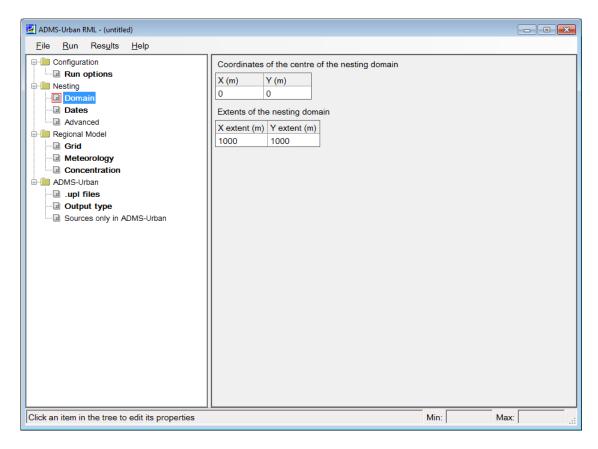


Figure 4.3 The **Domain** screen in the **Nesting** section of the ADMS-Urban RML Controller interface

4.2.1.1 Coordinates of the centre of the nesting domain

Enter the x and y coordinate values for the centre of the desired nesting domain, in a projected coordinate system consistent with that used to define the regional model grid. As in ADMS-Urban, all coordinate values must be entered in metres.

4.2.1.2 Extents of the nesting domain

Enter the extents of the nesting domain in the x and y directions, in units of metres.

4.2.2 Dates

The first and last hours of the modelling period are defined in the **Dates** screen, which is shown in **Figure 4.4**. Each item on the screen is described in Sections 4.2.2.1 to 4.2.2.2.

If a modelling period longer than the available regional model data is defined, the output will be restricted to the period when regional model data are available. The last hour may be equal to the first hour if the mixing time is set to one hour, if the mixing time is longer, the minimum number of hours which can be run is (mixing time -1) hours.

Note that the dates and times in the **Dates** screen should be defined in local solar time, as used in ADMS-Urban.

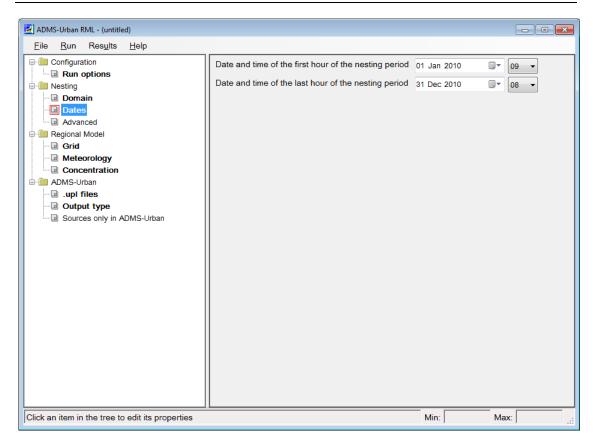


Figure 4.4 The **Dates** screen in the **Nesting** section of the ADMS-Urban RML Controller interface

4.2.2.1 Date and time of the first hour of the nesting period

Select the date and time of the first hour of the nesting period using the calendar and lists.

4.2.2.2 Date and time of the last hour of the nesting period

Select the date and time of the last hour of the nesting period using the calendar and lists. If a modelling period of a single hour is desired, the first and last date and time should be set to the same values. The difference between the first and last date and time must be at least (mixing time -1) hours, so a single hour can only be run if the mixing time is set to one hour.

4.2.3 Advanced

The **Advanced** screen of the **Nesting** section includes parameters which may be adjusted by users if required for their particular modelling scenario but for which the default values are likely to be adequate in most circumstances. The screen is shown in **Figure 4.5**. Each item on the screen is described in Sections 4.2.3.1 to 4.2.3.3.

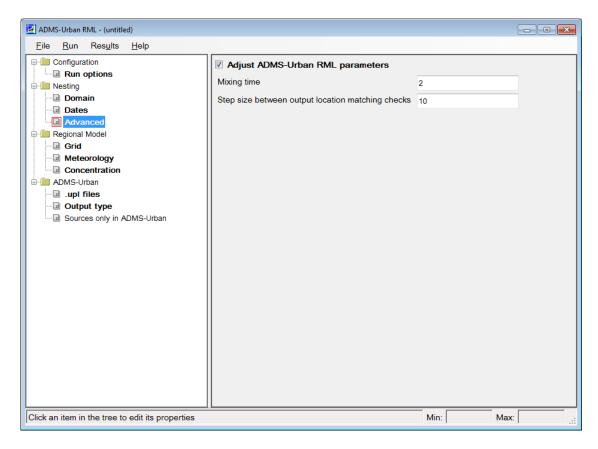


Figure 4.5 The Advanced screen of the Nesting section of the ADMS-Urban RML

Controller interface

4.2.3.1 Adjust nesting parameters

Click in this box to enable editing of the advanced nesting parameters.

4.2.3.2 Mixing time

The mixing time, T_m , is used to define the division of dispersion calculations between the regional model and ADMS-Urban in the ADMS-Urban RML system. In general, its value could depend on the regional model grid resolution and the meteorological conditions, however in practice a standard value of one or two hours has been found to be adequate. The default value of T_m in the ADMS-Urban RML system is one hour.

Longer values of T_m may be required if the regional model grid resolution is low (greater than ~3 km), as in this case it may take longer for explicitly modelled emissions to become well-mixed at the scale of a regional model grid cell, especially in low wind speed conditions. The mixing time must be defined as a whole number of hours. Please refer to Section 8.1 for more information about the role of the mixing time in the ADMS-Urban RML system.

4.2.3.3 Step size between output location matching checks

The calculation of nested output concentrations requires ADMS-Urban output from runs with gridded and explicit emissions at exactly matching output locations. The locations are checked by the **RML Output** utility to ensure that they match to within a

suitable tolerance. If an ADMS-Urban RML system run includes a large number of output points, it may be desirable to increase the step size between checks in order to reduce the RML Output utility run times. If **Grid for contouring** is chosen as the **Output type option** (refer to Section 4.4.2 for more details), the RML Controller enforces matching output locations in the runs with gridded and explicit emissions by using the same .asp file in both runs, so the step size can be set to a large number. Conversely, if the **Receptor locations** output type is chosen, the RML system will retain the user-specified output locations for each run and the step size should be left as its default value of 1.

4.3 Regional Model

The **Regional Model** section of the ADMS-Urban RML Controller interface contains information about the regional model meteorology and concentration data files to be used in the ADMS-Urban RML system. If you are using regional model data files obtained from a third party provider, you may need to obtain some additional information about the runs in order to fill in this section of the interface.

4.3.1 Grid

The **Grid** screen is used to define the regional air quality model grid, including its spatial location and resolution. The screen layout is shown in **Figure 4.6**. Each item on the screen is described in Sections 4.3.1.1 to 4.3.1.3.

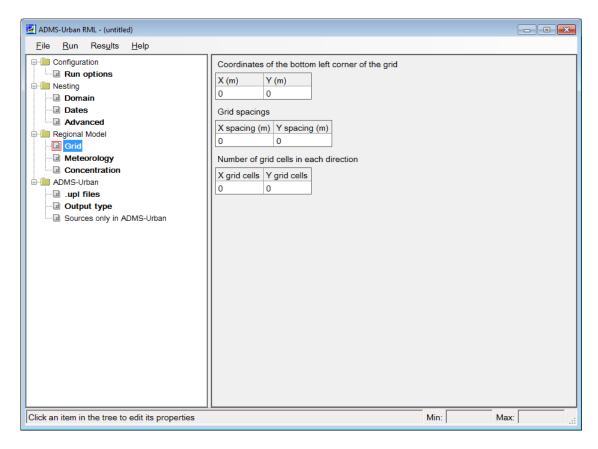


Figure 4.6 The **Grid** screen in the **Regional Model** section of the ADMS-Urban RML Controller interface

4.3.1.1 Coordinates of the bottom left hand corner of the grid

Enter the x and y coordinates of the bottom left corner of the regional air quality model grid, in projected coordinates with units of metres. If you are using output files from the CMAQ or CAMx regional models in IOAPI format, these coordinates can be obtained from the values of the XORIG and YORIG attributes.

4.3.1.2 Grid spacings

Enter the grid spacings of the regional model in the x and y directions, in units of metres. The regional model grid spacing is required to be uniform, ie. constant throughout the grid, but the x and y spacings may differ from each other. If you are using output files from the CMAQ or CAMx regional models in IOAPI format, these spacings can be found from the values of the XCELL and YCELL attributes.

4.3.1.3 Number of grid cells in each direction

Enter the number of regional model grid cells in the x and y directions (columns and rows respectively). If you are using output files from the CMAQ or CAMx regional models in IOAPI format, these numbers can be found from the values of the NCOLS and NROWS attributes.

4.3.2 Meteorology

The **Meteorology** screen contains information about the regional meteorological model data used to run the regional air quality model and to be extracted for use in ADMS-Urban within the RML system. At present, only output from the WRF model is supported by the system. If you have output data from a different meteorological model, it will need to be re-formatted into WRF output format for use in the ADMS-Urban RML system. The **Meteorology** screen is shown in **Figure 4.7**. Each item on the screen is described in Sections 4.3.2.1 to 4.3.2.5.

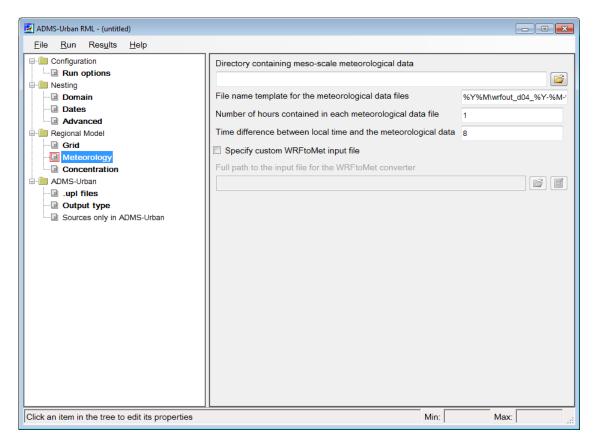


Figure 4.7 The **Meteorology** screen in the **Regional Model** section of the ADMS-Urban RML Controller interface

4.3.2.1 Directory containing meso-scale meteorological data

The file paths for regional model output files often include date and time information.

The location of the files is specified in two parts in the ADMS-Urban RML Controller interface:

- a date-independent directory path; and
- a date and/or time-dependent file path template which may also include any date or time-dependent directory structure components.

Please refer to the following section for details of the template file path format and an example of the path definitions. Click on the **Browse** button () to select the date-independent directory used to store the WRF output files.

4.3.2.2 File name template for the meteorological data files

The use of a file name template enables the ADMS-Urban RML Controller to generate file paths for regional model output for a specific date and time according to the defined pattern. The template is defined using 'tags', which consist of a percent sign (%) and a single letter, to indicate particular date or time components, for example %Y is used to represent a four-digit year value. A full list of currently available tags with example values for two dates is given in **Table 4.2**.

The following example shows a typical directory and file name structure for hourly WRF output files:

where the terms in angle brackets indicate a numerical value, such that the path for the file containing data for 1 am on 1st January 2014 has file path

This directory and file name structure would be entered into the ADMS-Urban RML Controller interface by selecting the date-independent directory

```
D:\WRF\run1\
```

and specifying the date-dependent file name template as

Note that the tag character is case-sensitive to distinguish between %M for month and %m for minute. The values for minute and second tags are always set to zero.

Tag	Description	Example values		
		1 am 1 st January 2014	2 pm 6 th March 2010	
%Y	Four-digit year	2014	2010	
%M	Two-digit month	01	03	
%D	Two-digit day of month	01	06	
%J	Three-digit Julian day	001	065	
%h	Two-digit hour	01	14	
%m	Two-digit minute	00	00	
% s	Two-digit second	00	00	

Table 4.2 Tags used to indicate date and time information in file name templates

4.3.2.3 Number of hours contained in each meteorological data file

Specify the number of hours of data included in each meteorological data file. At present, the number of hours of data included in each meteorological data file must be one.

4.3.2.4 Time difference between local time and the meteorological data

Enter the time difference between local solar time, as used in ADMS-Urban, and the time zone used in the meteorological model data files, in whole hours. Regional models are often run in a standard time system such as UTC, whereas ADMS-Urban runs in local solar time. For example, if meteorological data are obtained with UTC times and the local solar time is UTC +8, as in Hong Kong, a value of 8 should be entered. Both positive and negative values of time difference are permitted.

If the local solar time for your modelling area is a non-integer number of hours different from the time zone used in the meteorological model data files, enter the nearest whole hour value for the time difference.

4.3.2.5 Specify custom WRFtoMet input file

Click in this box if you wish to specify your own input file with non-default settings for the utility which extracts ADMS format met data from WRF files. When this option is selected, browse to a suitable input file using the **Browse** button (). The input file format for this utility is defined in Section A.3. The default input file can be found in a sub-directory of the ADMS-Urban RML Controller install directory, by default <*install_path*>\Data, and may be used as a template when creating a custom input file. Click the **Edit** button () to view or edit the currently selected file in Notepad.

Any user-edited input file for the WRF met extraction utility must not be saved in the ADMS-Urban RML Controller install directory.

At least one of solar radiation and surface sensible heat flux must be selected for extraction from WRF in order to create valid .met files for use in ADMS-Urban.

4.3.3 Concentration

The **Concentration** screen contains information about the regional air quality model output files. Many of the options are similar to those available for the meteorological data files. The **Concentration** screen is shown in **Figure 4.8**. Each item on the screen is described in Sections 4.3.3.1 to 4.3.3.8.

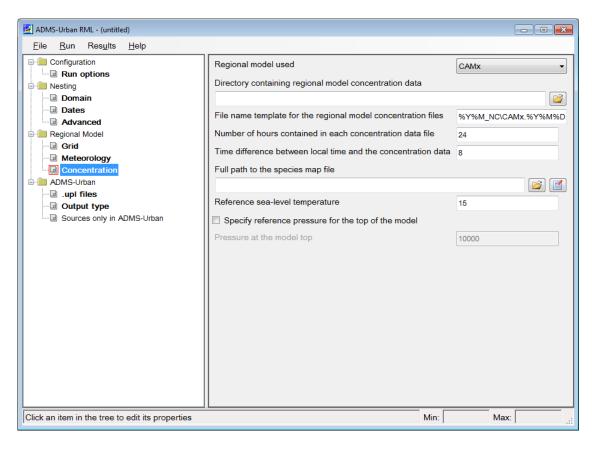


Figure 4.8 The **Concentration** screen in the **Regional Model** section of the ADMS-Urban RML Controller interface

4.3.3.1 Regional model used

Select the regional model from which concentration output files are available from the list. Currently available options are CAMx, CMAQ and EMEP4UK. CAMx output files must be converted into the IOAPI format, for example using the CAMxtoIOAPI utility, for use in the ADMS-Urban RML system. Any other regional model data which can be converted into IOAPI format could be used by selecting either of the CMAQ or CAMx options.

4.3.3.2 Directory containing regional model concentration data

Select the date-independent directory containing the regional model concentration data files using the **Browse** button. Please refer to Sections 4.3.2.1 and 4.3.2.2 for more details of the specification of date-independent directory path and date-dependent file name template, which are the same for both the meteorological and concentration data files.

4.3.3.3 File name template for the regional model concentration files

Specify the file name pattern including date and time information using tags as described in **Table 4.2**. Please refer to Section 4.3.2.2 for more details of the file name template conventions.

4.3.3.4 Number of hours contained in each concentration data file

Enter the number of hours of concentration data contained in each regional model concentration file. For example, if a separate regional model data file is created for each modelled day, a value of 24 should be entered.

4.3.3.5 Time difference between local time and the concentration data

Enter the time difference between the local solar time, as used in ADMS-Urban, and the time zone used in the regional air quality model output files, in whole hours. Regional models are often run in a standard time system such as UTC, whereas ADMS-Urban runs in local solar time. For example, if concentration data are obtained with UTC times and the local solar time is UTC +8, as in Hong Kong, a value of 8 should be entered. Both positive and negative values of time difference are permitted.

4.3.3.6 Full path to the species map file

The species map file is used to link regional model chemical species to ADMS-Urban chemical species. Select the desired input species map file using the **Browse** button (). Click the **Edit** button () to view or edit the currently selected file in the application selected in the **File**, **Preferences**... menu, by default Notepad. An example species map file is shown in **Figure 4.9**.

The columns in the species map file each represent an ADMS-Urban species, and the rows a regional model species. The values in the matrix are conversion factors, such that the concentration C_i of ADMS-Urban species i in $\mu g/m^3$ is given by:

$$C_i = \sum_{j=1}^{n_{RM}} S_{ij} C_j$$

where n_{RM} is the number of regional model species j, S_{ij} is the species map conversion factor from regional model species j to ADMS-Urban species i, and C_j is the regional model concentration of species j. Most of the species map values are 0, but this approach allows:

- regional model species to be part of more than one ADMS-Urban lumped species, for example all PM_{2.5} component species also contribute to PM₁₀;
- unit conversion factors to be specific to the ADMS-Urban species, for example the NO contribution to NO_x as NO₂ would have a different conversion factor to NO as an explicit species; and
- ADMS-Urban lumped species to have an arbitrary number of components, for example ten regional model species contribute to ADMS-Urban PM₁₀, but only one to O₃.

Note that the species map conversion factors should include an appropriate unit conversion to $\mu g/m^3$ for all species.

ADMS-Urban and regional model species names should be given exactly as used in the models, including capitalisation.

Saving the species map file from Excel in .csv format may lead to extra commas at the end of the header lines.

The structure of the species map file, which should be saved as a comma-separated text file (.csv), is as follows:

Version string: 'SPECIESMAPVERSION1'

Number of output (ADMS-Urban) species

Number of input (Regional model) species

Header line: 'Variables' followed by comma-separated list of names of all output species (as used in ADMS-Urban)

Data lines: Name of an input species (matching the species variable name used in the regional model netCDF output files), followed by a comma-separated list of multiplying factors for how much of this input species should be added to each output species, including unit conversions to $\mu g/m^3$ where necessary.

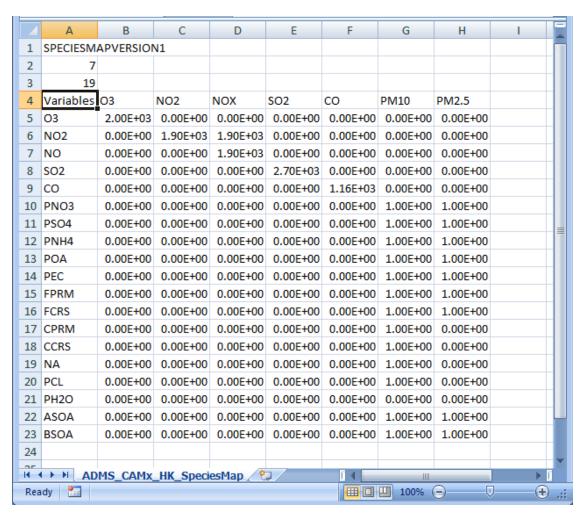


Figure 4.9 Example species map file viewed in Excel

4.3.3.7 Reference sea-level temperature

Enter a standard sea-level temperature for the modelling domain in degrees Celsius. The RML Output utility, which is used to calculate the nested output concentrations, selects the appropriate regional model vertical grid layer by converting the layer sigma coordinate values into heights. This requires a standard value of sea-level temperature, for example an annual or period average for the modelling domain. Please refer to Section C.2 for further details of the procedure for calculating regional model grid heights.

4.3.3.8 Specify reference pressure for the top of the model

The reference pressure at the top of the regional model grid is also required to calculate regional model heights from sigma layer values. By default the ADMS-Urban RML Controller will obtain the pressure at the top of the regional model grid from the concentration output files. However, this value may be incorrect if the output has been re-formatted. Select **Specify reference pressure for the top of the model** to override the model-top pressure found in the regional model concentration output files. Enter the correct value in Pascals.

If you are using output files from the CMAQ or CAMx regional models in IOAPI format, the model top pressure can be found from the value of the VGTOP attribute. In WRF files the model top pressure can be found from the value of the P_TOP variable. These variables should have consistent values.

4.4 ADMS-Urban

The ADMS-Urban section of the RML Controller interface contains options relating to the ADMS-Urban runs used in the ADMS-Urban RML system.

4.4.1 .upl files

The .upl files screen in the ADMS-Urban section of the ADMS-Urban RML Controller interface contains file paths for the three ADMS-Urban model parameter files (.upl extension) used in the ADMS-Urban RML system. The .upl files screen is shown in Figure 4.10. Please refer to the ADMS-Urban User Guide for general information about how to create .upl files. A brief description of the three .upls and their roles in the ADMS-Urban RML system is given in Section 1.3, more details can be found in the technical summary, Section 8.2.

For each .upl, the RML Controller will apply appropriate spatial and temporal truncation for each regional model grid cell covered by the nesting domain and substitute the .met and .bgd file paths corresponding to the relevant cell, please refer to Section 8.5.1.1 for more information.

The main differences between the three .upl files used in the ADMS-Urban RML system are the sources which they contain:

• the .upl with gridded emissions for the nesting background run contains gridded emissions matching those used in the regional model;

- the .upl with explicit emissions for the main nesting run contains emissions at the highest known resolution, which may include both explicitly defined road and point sources and gridded sources for minor road or domestic heating emissions; and
- the .upl with gridded emissions for the main nesting run contains emissions equivalent to those in the .upl with explicit emissions, but all defined as gridded sources.

All three .upls should include the same Meteorology and Background settings. There are differences in the permitted and recommended settings for Setup, Grids and Output for the three runs. Common aspects for all three runs are discussed below, while settings specific to a particular .upl are discussed in Sections 4.4.1.1 to 4.4.1.3.

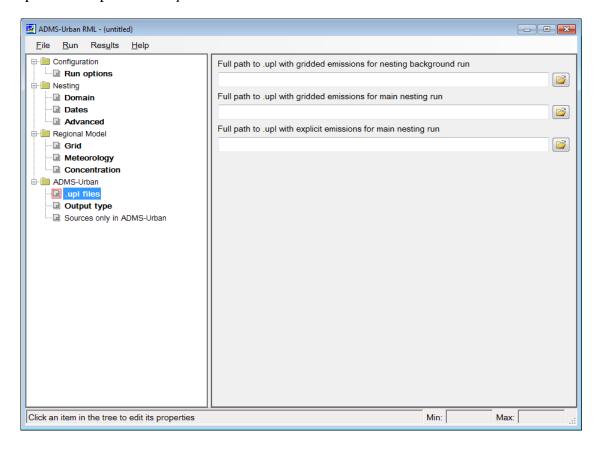


Figure 4.10 The .upl files screen in the ADMS-Urban section of the ADMS-Urban RML Controller interface

Setup

If you wish to include the effects of deposition in the locally-modelled concentrations, select the **Dry deposition** and/or **Wet deposition** option(s). Note that the ADMS-Urban RML system is currently only set up to calculate nested concentration values, not deposition, so no deposition rates will be included in the final outputs.

The **Odours** and **Buildings** options are not currently permitted in the ADMS-Urban RML system.

If you wish to model NO_x chemistry, or the contribution of SO_2 to particulate concentrations, select the **Chemistry** option, click on the **Enter parameters**... button and

select the Chemical reaction scheme option.

The Trajectory Model, which is used in standard ADMS-Urban modelling to take into account long-range chemical effects for distant grid source cells, should not be used in the ADMS-Urban RML system .upls as these effects are captured by the regional model chemistry.

The **Complex terrain** option should not be used in the .upl with gridded emissions for nesting background, as the meteorology extracted from the meso-scale meteorological model will include complex terrain effects at the resolution used by the regional air quality model.

The **Complex terrain** option should only be considered for use in the main nesting .upl files (gridded and explicit emissions) if all three of the following conditions can be satisfied:

- the nesting domain is significantly smaller than the corresponding meteorological model domain;
- terrain elevation and/or roughness length data are available for the modelling region at significantly higher resolution than the regional meteorological model grid resolution; and
- the complex terrain modelling resolution selected in the ADMS-Urban interface corresponds to a higher grid resolution across the terrain or roughness file extent than was used in the regional meteorological model.

Use of the ADMS-Urban **Complex terrain** module may lead to inconsistent nesting results, as local meteorological data from the current meteorological model grid cell is used as 'upstream' input to the whole area covered by the terrain or roughness file data, so should be treated with extreme caution.

Source groups

No user-defined groups should be defined in the run with gridded emissions for nesting background. User-defined groups may be defined in the main nesting runs, but only the output from the first group in the output netCDF files, which will be the **All Sources** group, will be used for the RML system output.

Meteorology

The **Met. measurement site** parameters, such as surface roughness, should be set equal to the **Dispersion site** parameters, as local meteorological data from the corresponding cell of the meteorological model will be used. The nesting domain latitude should be defined. The **Dispersion site Surface roughness** and any advanced options should be set based on the corresponding values used in the meso-scale meteorological model.

The RML Controller will supply the file path of a .met file extracted from the regional model meteorological data for the relevant grid cell at run time, so any .met file specified in the .upl file will not be used. The met data extracted from the WRF output does not have wind directions in sectors and is always hourly sequential.

The Use a subset of met. data option should not be selected, as the ADMS-Urban RML

Controller will set this as required by the dates given in the RML Controller interface.

Vertical profile data are not currently extracted from WRF for use in the ADMS-Urban RML system.

Background

A background concentration file containing local upwind background from the regional model is supplied by the ADMS-Urban RML Controller, so any .bgd file specified in the .upl file will not be used. If the **Chemistry** option is selected, either **From** file or **Enter by hand** must be selected on the **Background** screen to allow the .upl file to be saved with output of non-emitted pollutants such as ozone (O_3) selected.

4.4.1.1 Full path to .upl with gridded emissions for nesting background run

Select the .upl file with gridded emissions for use in the nesting background run using the **Browse** button (). This .upl should have emissions matched as closely as possible to those used in the regional model, in both magnitude and time-variation. Details of the recommended input options which differ from those in the other .upl files are given below, arranged in the order of the main screens of the ADMS-Urban interface.

Setup

If including **Dry Deposition** or **Wet Deposition** in this run, ensure that pollutant deposition parameters are set to match those used in the regional model.

No additional input file (.uai) should be supplied for this run.

Sources and emissions

This .upl should include only gridded emissions, with no explicit sources, in order to match the behaviour of the regional model as closely as possible. Gridded emissions should be defined to cover the whole of the selected nesting domain. A larger extent of emissions may be defined in the .upl file, for example covering the whole of the regional model domain, as the emissions will be spatially truncated to the extents of each regional model grid cell within the nesting domain before running.

The grid source should be defined with horizontal geometry matching the regional model horizontal grid definition, and depth equal to twice the height of the regional model grid layer(s) containing the majority of the ground-level emissions. For example, if the lowest regional model grid layer is 20 m deep and contains 95% of the emissions from non-point sources, an ADMS-Urban grid source depth of 40 m would be suitable. The doubling of the grid source depth ensures that ADMS-Urban uses velocity and turbulence parameters from the boundary between the lowest two regional model grid layers for dispersion modelling, in order to match the regional dispersion model. This is most important for regional models with high vertical grid resolution close to the ground; if the near-ground grid resolution is coarse, for example a lowest grid layer thickness of 50 m or more, the doubling of the ADMS grid depth may not be necessary due to the shallower gradients of flow and dispersion parameters at this height.

The magnitude of the emission rate in each grid cell should correspond to the annual average emission from the corresponding regional model grid cell. Note that unit and species conversions may be required to obtain emissions suitable for an ADMS-Urban grid source from those used in the regional model.

Any time-variation used in the regional model emissions should be included in this .upl file using either a .fac file or hourly factors specified in the ADMS-Urban interface. The .fac file allows monthly profiles to be included in addition to daily variation on weekdays, Saturdays and Sundays or each day of the week. If different time-varying profiles are used for different source types in the regional model, a weighted average profile should be calculated for use in ADMS-Urban.

Poor matching between the emissions used in this run and the regional model emissions can lead to invalid nesting background calculations. If large numbers of negative nesting background hours are reported as warnings from the RML Background utility, the emission factors and time-variation profiles used in this run should be assessed for consistency with those used in the regional model.

Grids

One specified output point should be defined in the centre of each horizontal regional model grid cell included in the nesting domain, at a height of half the thickness of the lowest grid layer in the regional model. An .asp file may be the most convenient way to set up these output points.

Output

An output should be defined for each ADMS pollutant listed in the species map file (described in Section 4.3.3.6). The outputs should be specified as:

- short-term (ST),
- units of $\mu g/m^3$ and
- averaging times of 1 hour.

The All sources group output option should be selected. A Comprehensive output file is not required from this run.

Other inputs

No additional model options are recommended in this run.

4.4.1.2 Full path to .upl with gridded emissions for main nesting run

In general this .upl should be identical to the .upl with explicit emissions, described in the following section, except that it does not include any explicit sources. Thus the easiest way to create this .upl is to make a copy of the .upl with explicit emissions and delete all the explicit sources. It is also advisable to remove any additional input options which only apply to explicit sources, such as the advanced street canyon module. Further modifications may be necessary if the .upl with explicit emissions includes any sources not included in the regional model emissions, for example from new developments, as emissions from these sources should not be included in this .upl.

Please refer to Section 4.4.3.1 for more details of how to model sources not included in the regional modelling.

Setup

Please refer to the *Other inputs* section below for a discussion of additional input (.uai) file options for this run.

Sources and emissions

If there are no sources included in the run with explicit emissions which were not included in the regional model emissions, this *.upl* should include exactly the same grid source emissions, in terms of magnitude and time-variation, as are included in the run with explicit emissions (described in Section 4.4.3.1). These may differ from the grid source emissions used in the run with gridded emissions for nested background, described in Section 4.4.1.1, for example if the road traffic emissions or time-variation have been re-calculated based on additional local data, or if gridded emissions data are available at higher resolution than were used in the regional model. For consistent results across a nesting domain which covers multiple regional model grid cells, it is recommended that the ADMS-Urban grid geometry fits exactly into the regional model grid cell geometry.

If there are sources included in the run with explicit emissions which were not included in the regional model emissions, for example a new or proposed development, this .upl should include the grid source emissions used in the run with explicit emissions, but with the emissions from the sources not included in the regional model subtracted.

Grids

If the **Receptor locations** output type has been chosen in the ADMS-Urban RML Controller interface, specified point locations should be defined which match those selected in the run with explicit emissions. If the **Grid for contouring** option is selected, the output locations specified in this run will not be used. Please refer to Section 8.3 for more details of the additional processes involved in the **Grid for contouring** option.

Output

An output should be defined for each ADMS pollutant listed in the species map file (described in Section 4.3.3.6). The outputs should be defined as:

- long-term (LT),
- units of μg/m³ and
- averaging times of 1 hour.

The All sources group output and Comprehensive output file options should be selected.

Other inputs

The Urban Canopy module may be specified via a .uai file for this run, if it will also be used in the run with explicit emissions.

4.4.1.3 Full path to .upl with explicit emissions for main nesting run

This .upl should be set up according to the best practice for local modelling with ADMS-Urban, with advanced modelling of road sources in street canyons if required.

Setup

Please refer to the *Other inputs* section below for a discussion of additional input (.uai) file options for this run.

Sources and emissions

Sources should be set up in this .upl according to the best available explicit and gridded emissions data. Please refer to the ADMS-Urban User Guide for information about the source types available in ADMS-Urban. Time-variation of emissions can be defined on a source-by-source basis if this information is available.

The grid source geometry should be the same as that used in the main nesting run with gridded emissions. The grid source emissions used in this run should include all the explicit emissions, so they may be different from those used in the main nesting run with gridded emissions if there are explicit sources in this run which are not included in the regional model emissions. They may also differ from the emissions used in the nesting background run if improved local emissions data are in use.

Grids

If the **Receptor locations** output type has been chosen in the ADMS-Urban RML Controller interface, specified point locations should be defined which match those selected in the main nesting run with gridded emissions. If the **Grid for contouring** option is selected, the output locations specified in this run and the explicit source locations will be used for the **Create ASP** run to allow the creation of an *.asp* file including source-oriented grid point locations. Please refer to Section 8.3 for more details of the additional processes involved in the **Grid for contouring** option, including the **Create ASP** mode ADMS-Urban run.

Output

An output should be defined for each ADMS pollutant listed in the species map file (described in Section 4.3.3.6). The outputs should be defined as:

- long-term (LT),
- units of µg/m³ and
- averaging times of 1 hour.

The All sources group output and Comprehensive output file options should be selected.

Other inputs

Any of the additional model options available in ADMS-Urban may be used in this run, for example the Urban Canopy flow field and/or street canyon modules. If you wish to alter the number and/or locations of source-oriented grid points for road or line sources (intelligent grid points), to improve the resolution of concentration contours, an .igp file can be created and specified in the .uai file for this run. Please refer to the ADMS-Urban User Guide for more details of the available .uai and/or .igp options.

4.4.2 Output type

The **Output type** screen in the **ADMS-Urban** section of the ADMS-Urban RML Controller interface allows the user to specify whether the RML system run output is for a small number of receptor locations, for example at monitoring sites for model validation purposes, or for a grid of locations which will be used to produce contours of concentration. In the latter case, additional procedures are included in the ADMS-Urban RML system to ensure that ADMS-Urban source-oriented and interpolated intelligent grid points are included in the final output, which allows high-resolution contour output to be produced. The **Output type** screen is shown in **Figure 4.11**. The input for this screen is described in Section 4.4.2.1.

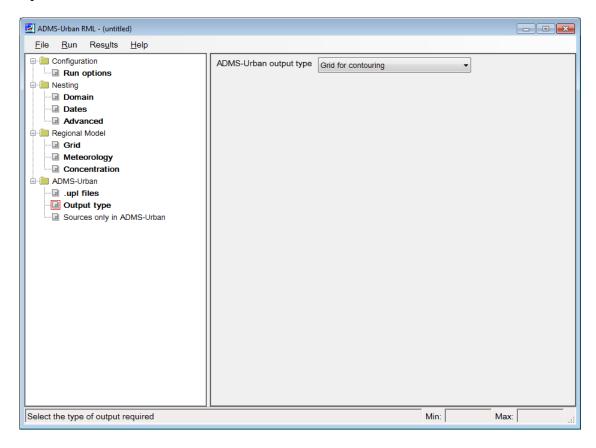


Figure 4.11 The **Output type** screen in the **ADMS-Urban** section of the ADMS-Urban RML Controller interface

4.4.2.1 ADMS-Urban output type

Select the output type of your ADMS-Urban RML system run from the list.

- Choose the **Receptor locations** option if your ADMS-Urban runs contain only specified points or do not include the **Source-oriented grids** option.
- Choose the **Grid for contouring** option if you want to produce high-resolution contour plots using the source-oriented grid points option.

Please refer to Section 8.3 for details of the additional procedures which are included in the RML system when the **Grid for contouring** option is chosen.

4.4.3 Sources only in ADMS-Urban

If the ADMS-Urban RML system is being used for an environmental impact assessment of a proposed development, the emissions for the new development are unlikely to be included in the regional air quality model emissions data. In this case, the emissions from the new development should not be subtracted from the regional model concentrations, and ADMS-Urban should be allowed to model them without truncation of the dispersion time. Please refer to Section 8.4 for more details of the treatment of sources only included in ADMS-Urban in the RML system.

The **Sources only in ADMS-Urban** screen of the ADMS-Urban RML Controller interface allows sources which should be treated in this way to be specified by name. The **Sources only in ADMS-Urban** screen is shown in **Figure 4.12**. The inputs to the screen are described in Sections 4.4.3.1 and 4.4.3.2.

The emissions from any sources not included in the regional modelling should only be included in the ADMS-Urban run with explicit emissions.

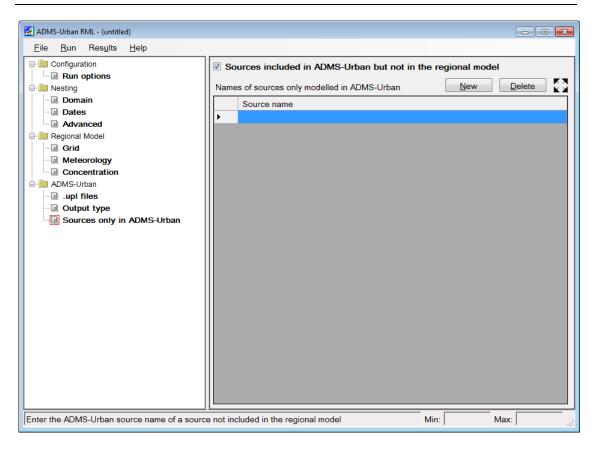


Figure 4.12 The **Sources only in ADMS-Urban** screen in the **ADMS-Urban** section of the ADMS-Urban RML Controller interface

4.4.3.1 Sources included in ADMS-Urban but not in the regional model

Select **Sources included in ADMS-Urban but not in the regional model** to specify that one or more sources have been included in the ADMS-Urban modelling which were not included in the regional modelling.

4.4.3.2 Names of sources only modelled in ADMS-Urban

Enter the names of any sources only modelled in ADMS-Urban in the table, with names exactly as used in ADMS-Urban. Click on the **New** button to add a row to the table. Multiple rows can be added at once by copying a list of source names to the clipboard, for example from a .csv file opened in Excel, right-clicking in a blank area of the screen and selecting **Paste**. Rows can be copied from the table by highlighting, right clicking and selecting **Copy**.

Use the **Delete** button to delete the currently selected row(s). Right click and select **Delete all** to delete all the currently defined rows.

The table can be expanded to fill the RML Controller interface window using the Full screen editing button (), or by right-clicking and selecting Full screen editing.

SECTION 5 ADMS-Urban RML system output

This section describes the outputs which are produced by the ADMS-Urban RML system and suggests methods for some common post-processing tasks. The main output files, which will be produced by all successful RML system runs, are an RML Controller log file and an ADMS format netCDF file containing concentration data, these are described in Sections 5.1.1 and 5.1.2 respectively. Other files which may be returned by the RML system are described briefly in Section 5.1.3.

Section 5.2 describes how to use ADMS utilities to extract statistics and plot contours of concentration from the ADMS-Urban RML system output file.

5.1 Output files

Note that the output files returned by the ADMS-Urban RML system at the end of a run will depend on the user's choice of RML Controller save options, as described in Section 4.1.1.1.

5.1.1 ADMS-Urban RML Controller log file

The ADMS-Urban RML Controller generates a log file which records each component activity of the RML system, with details of the inputs and whether the component ran without errors. The log file is a text file with the same file name stem as the input .npl file, with the extension .log. The log file from a previous run of the RML system with the .npl currently open in the interface can be accessed from the ADMS-Urban RML Controller interface by clicking on Results, View log file, which will open the log file in the application specified in the Viewing tab of the File, Preferences... screen, by default Notepad.

The beginning of the log file gives details of the RML Controller system component version numbers and the ADMS-Urban RML licence which is in use. This information may assist with investigating any issues with the system.

Each entry in the main section of the log file consists of date and time information, followed by a message about the current stage of the RML system. For example, a call to the utility which extracts meteorological data from WRF would be recorded as follows:

15/07/2014 18:08:44: Launched utility WRFToMet with command line 2010 04 01 9 2160 "D:\Controller\Working\18500_-665000\18500_-665000MetData.met" 2 18500 - 665000

A summary is given at the end of the .log file of the number of regional model grid cells included in the nesting domain and whether they ran without errors, for example, for a receptor locations run where the nesting domain covered 968 but only 13 contained receptors the summary shown in **Figure 5.1** was obtained.

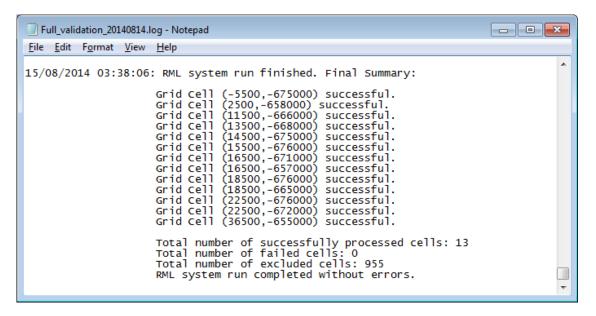


Figure 5.1 Summary section of an ADMS-Urban RML Controller log file

'Excluded cells' are regional model grid cells which do not include any output points, whereas 'failed cells' are cells which do include at least one output point but where some error has occurred during the RML system run.

5.1.2 RML system final output file

The concentrations output by the ADMS-Urban RML system are stored in a netCDF (.nc) file which follows the ADMS Comprehensive Output File conventions. This format is described in full in the ADMS-Urban User Guide.

There is a dedicated utility for processing these files, the ADMS Comprehensive Output File processor, which allows the user to view the raw concentration data, calculate statistics and export concentration data to ADMS format text files. Click **Results, Extract statistics...** to open the .nc file from the currently selected .npl in the ADMS Comprehensive Output File Processor. Please refer to the ADMS Comprehensive Output File Processor User Guide (CERC, 2014c) for more details of the available processing options.

5.1.3 Intermediate files

The number and type of intermediate files retained by the ADMS-Urban RML Controller depends on the *.npl* setting for RML Controller save options, which is described in Section 4.1.1.1.

Intermediate files are stored in a directory created with the file-name stem of the .npl file, appended with '- other files' within the directory where the .npl file is saved. For example, if your .npl file is $D:\My\ Work\Test.npl$ then the intermediate files would be saved in $D:\My\ Work\Test-$ other files\.

Within this directory, additional directories will be created for each regional model

grid cell included in the nesting domain if it includes any output points, named according to the x and y coordinates of the centre of the grid cell. For example, if your nesting domain covers the region (0, 0) to (2000, 2000), with regional model resolution of 1000 m, all files associated with the lower-left cell of the domain would be filed in $D:\My\ Work\Test-other\ files\500_500\$. If the option to save all files is chosen, a directory will be created for every regional model grid cell included in the nesting domain.

If the mixing time used in the RML system is greater than one hour, the main ADMS-Urban runs, which are repeated for each hour of the mixing time, are filed in subdirectories of the grid cell directories, named according to the hour of the mixing time. For example, the run with truncation from 0 to 1 hour for the lower-left cell of the domain described above would be filed in $D:\My \ Work\Test - other files |500_500|0|$.

Each ADMS-Urban run within the ADMS-Urban RML system produces standard ADMS-Urban output files, for example *.mop, *.log. Please refer to the ADMS-Urban User Guide for details of the formats and contents of these files. The input and output files associated with each of the RML Controller utility programs are described in the Appendices.

Strict naming conventions are used by the RML Controller to ensure that every file has a unique name without an excessively long file path. **Table 5.2** shows the file naming conventions used for each stage of the ADMS-Urban RML system.

Error or warning files created by the RML Controller utilities use a slightly different convention, according to *TypeComponentXC_YC* where *Type* may be Error or Warning, *Component* matches the utility file name stem shown in **Table 5.2** and *XC_YC* are the grid cell centre coordinates. This allows all warning or error files to be identified rapidly within a directory which may contain a large number of files.

Stage	Interface inputs	Description	File name stem	Each cell?	Each hour of Tm?
Step 2	4.4.1.3	Initial checking ADMS- Urban runs	XC_YCInitialCheck	Y	N
Step 3	4.3.2	Extraction of met data	XC_YCMetData	Y	N
Step 4		Extraction of local upwind background	XC_YCLocalUpwind	Y	N
Step 5	4.4.1.1	ADMS-Urban run for nesting background	XC_YCBgdGrid	Y	N
Step 6		Calculation of nesting background	XC_YCNestingCalc	Y	N
Step 7	4.4.1.2	Main ADMS-Urban runs: gridded emissions	XC_YCMainGrd or \H\XC_YCMainGrdH	Y	Y
Step 7	4.4.1.3	Main ADMS-Urban runs: explicit emissions	XC_YCMainExpl or \H\XC_YCMainExplH	Y	Y
Step 8		Calculate nesting output concentrations	XC_YCRMLOutput	Y	N
Step 9		Combine output files	CombineOptInput and Complete	N	N
(8.3.1)	4.4.1.3	Create .asp file with source-oriented grid locations	CreateAsp	N	N
(8.3.2)		Add interpolated source- oriented grid points	Complete.out	N	N

Table 5.2 Summary of file naming conventions used in the ADMS-Urban RML system. Please refer to Section 8.2 for a detailed description of each Stage, or to Section 8.3 for the additional procedures used to produce high-resolution contour output. Please refer to the sections in the Interface inputs column for information about corresponding RML Controller interface inputs. XC and YC represent the central x and y coordinates of the centre of the grid cell, and H each hour of a mixing time greater than 1 hour, starting from 0. The 'Each cell?' and 'Each hour of Tm?' columns indicate whether files are created for each regional model grid cell covered by the nesting domain and/or each hour of a mixing time greater than 1 hour, respectively.

5.2 Output file processing

5.2.1 Extract statistics

From the ADMS-Urban RML Controller interface, click **Results**, **Extract statistics**... to open the .nc file from the currently selected .npl in the ADMS Comprehensive Output File Processor. Select **Create Output** to open a screen where you can choose which output types, pollutants and output averaging times to use, then click **Create Files** to obtain the output text files. Please refer to the ADMS Comprehensive Output File Processor User Guide (CERC, 2014c) for more details.

If a .pst file is extracted from the RML system output file, this can be used as input to the MyAir Model Evaluation toolkit in order to compare nested concentrations to

measured values. Please refer to the MyAir Model Evaluation Toolkit User Guide (CERC, 2013b) for more details.

5.2.2 Plot contours of concentration

Use the ADMS Comprehensive Output File Processor **Create Output** function to extract a .gst or .glt file from gridded and source-oriented grid output locations in the ADMS-Urban RML system .nc output file. This text file can then be used to create concentration contours in the ADMS Mapper, Surfer, ArcGIS or MapInfo using the ADMS Contour Plotter. Please refer to the ADMS-Urban User Guide (CERC, 2014a) for more information about the ADMS Contour Plotter and the ADMS Mapper User Guide (CERC, 2013a) for more information about the ADMS Mapper.

SECTION 6 Troubleshooting

This section gives guidance on how to investigate common errors from the ADMS-Urban RML system. Section 6.1 gives tips for improving the appearance of high-resolution contour plots. Section 6.2 outlines a procedure for investigating cells which are reported as 'failed' by the RML Controller. The remaining errors are arranged according to the component of the RML system from which they would be issued or with which they are associated. This is not a comprehensive list of errors which can be issued by all components of the RML system if run as stand-alone utilities, as the RML Controller ensures correct settings for many inputs.

6.1 Tips for creating high-resolution contour plots

Users are strongly advised to run the ADMS-Urban RML in model verification mode and create a test plot of the output before starting a large contour run for a long modelling period. This will allow you to ensure that the output grid settings are suitable for high-resolution concentration contours. The following problems may be encountered:

Problem 1: The contour boundaries are uneven, particularly near the boundaries between regional model grid cells.

Solution 1: If using the Kriging method for creating contours, ensure that the nominal grid spacing reflects a resolution intermediate between the regular grid spacing and the source-oriented grid point spacing. In addition, when defining a regular output grid in ADMS-Urban, ensure that it is offset from regional model grid cell boundaries and has spacing smaller than the regional model grid resolution, so that there are a consistent number of output points per regional model grid cell, ideally at least 10 points in each direction.

Problem 2: The contour resolution is poor near the explicitly-modelled road sources

Solution 2: View the locations of the output points used as input to the contour process. There should be output points along each of the explicitly-modelled road sources. If the output points near roads do not form a high-density network, define an .igp file with an increased maximum number of source-oriented grid points for road sources and apply it to the .upl with explicit emissions via a .uai file.

6.2 Investigating failed cells

If the RML Controller summary of the run indicates that one or more cells have failed, the following steps will help to identify the cause of the failure:

You may wish to select a different RML Controller directory or rename the working directory and create a new one before investigating failed cell(s), so that the working files for the run with the failed cell(s) are not overwritten during the investigation.

• Open the RML Controller < run name > .log file from the run in a text editor, such as

Notepad.

- Search the file for the word 'failed' (without the inverted commas). Note which cell(s) have failed, eg. "-15500_-678000" and at which stage of the RML system run, eg. RML Output.
- For each failed cell:
 - * Open the *<run name> other files* directory and identify the subdirectory for the failed cell.
 - * Open any Error file for the failed stage in a text editor, which can be identified following the naming conventions described in **Table 5.2**. The contents of the file will give additional information about which stage of the ADMS-Urban RML system failed for this cell.
 - * If there is no error file or the error does not have an obvious cause, try re-running the failed stage manually, either by manual submission of an ADMS-Urban run to Run Manager or by following the Appendix instructions for running the relevant utility program, to see whether the error is repeated. If you have not chosen to keep all files, the input files for the failed stage can be found in the cell's subdirectory of the RML Controller working directory. If the error is not repeated when the failed stage is re-run, it may have been caused by a temporary problem, for example an interruption in the network connections between PCs used by the ADMS-Urban RML. If the error is repeated and you cannot identify its cause, contact the CERC helpdesk for support.
- Once you have corrected the error(s) and re-run the failed stage for each failed cell, consider re-running the remaining stages of the ADMS-Urban RML manually, following the instructions given in the Appendices, or re-running the complete ADMS-Urban RML run. If a cell has failed in the initial stages of the ADMS-Urban RML run, ie. before the main ADMS-Urban runs have been performed, it is likely to be necessary to rerun the complete system run. However, if a cell has failed during the main ADMS-Urban runs or one of the post-processing stages, re-running the failed stages manually may be less time-consuming.

6.3 RML Controller

Errors from the ADMS-Urban RML Controller are by default issued to pop-up message boxes on the screen, although this behaviour can be suppressed using an option in the configuration (.ini) file, please refer to Section 2.2.3 for details.

Note that error message boxes can appear behind the main RML Controller progress window. If the progress window appears to stall with no error text, try minimising the progress window to check whether there is an error box behind.

Errors from the ADMS-Urban RML Controller are also written to the ADMS-Urban RML Controller .log file, which is output to the directory of the input .npl file.

Errors from ADMS-Urban runs or RML Controller utility programs are copied to the ADMS-Urban RML system progress window, in addition to appearing in the relevant log and/or error files.

6.3.1 Run Manager Central Repository



Figure 6.1 Browse screen displayed if the Run Manager Central Repository location has not been set in the ADMS-Urban RML Controller interface

Problem 1: If the Run Manager Central Repository location has not been set in the ADMS-Urban RML Controller interface, when the RML system is run a Browse screen will be displayed, allowing the user to select the Run Manager repository location, as shown in **Figure 6.1**. The ADMS-Urban RML system run cannot proceed without a valid Run Manager repository path.

Solution 1: Browse to a valid Run Manager Central Repository directory

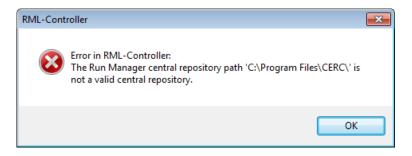


Figure 6.2 Error message for invalid central repository path

Problem 2: **Figure 6.2** shows the error message which will be issued if a Run Manager repository location has been set which does not exist or is not a Run Manager repository.

Solution 2: Check the Run Manager repository setting using File, Change Run Manager repository from the ADMS-Urban RML Controller interface. Refer to Section 2.2.3 for details of how to set the repository location or to the Run Manager User Guide (CERC, 2014b) for more details about the Run Manager central repository.

6.3.2 Run Manager Model name or Execution Group name

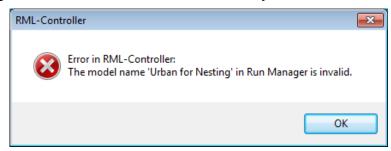


Figure 6.3 Example error message for invalid Run Manager model name

Problem: **Figure 6.3** shows an example of an error message which will be issued if the model name or execution group in Run Manager is invalid. These messages indicate that the entries for **Model name in Run Manager** or **Execution group to use in Run Manager** on the **Configuration, Run options** screen of the ADMS-Urban RML Controller interface are incorrect.

Solution: Check that the entries in the ADMS-Urban RML Controller interface exactly match the spelling, capitalisation and punctuation of the model name and execution group as shown on the **Add Runs** screen in Run Manager.

6.3.3 Nesting domain not covered by regional grid cells

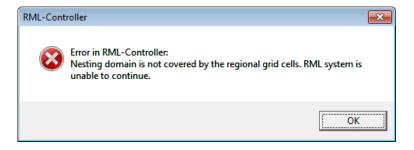


Figure 6.4 Error message for incorrect nesting domain settings

Problem: **Figure 6.4** shows the error message which will be issued if the nesting domain coordinates are not fully within the extents of the regional model grid, as specified in the *.npl*.

Solution: Check that the same coordinate system has been used to define both the regional model grid and the nesting domain centre and extents.

6.3.4 Manual retrieval of run files

Problem: A network failure between the RML Controller machine and the location of the *.npl* directory may lead to run files not being returned to the *.npl* directory at the end of an otherwise successful ADMS-Urban RML system run (Step 10 of the RML system procedures described in Section 8.2).

Solution: Output files and some input files will be stored in the ADMS-Urban RML Controller working directory up to the start of any subsequent RML system run, and can be manually retrieved. The files which are stored depend on the RML Controller save options setting in the .npl:

- All files all input and output files from every stage of the RML system will be stored in the working directory; and
- Log files only or Key files the key files will be stored in the working directory for both of these settings.

Please refer to Section 4.1.1.1 for more details of **RML Controller save options** and key files.

6.4 ADMS-Urban model

Errors from ADMS-Urban model runs are written to the ADMS-Urban .log file, in the same directory as the relevant .upl file. All ADMS-Urban model runs in the RML system are carried out with spatial truncation to a single regional model grid cell, except the run in **Create ASP** mode if the **Grid for contouring** output type option is selected. Hence the .upl files and associated .log files are stored in directories for each grid cell, as described in Section 5.1.3.

6.4.1 Spatial truncation removes all output points

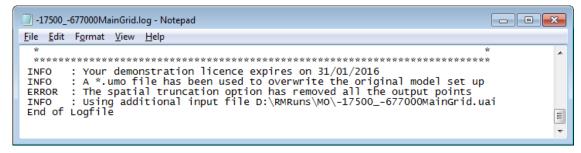


Figure 6.5 Example error message if no output points are within the spatial truncation limits.

Problem: ADMS-Urban will stop with an error if there are no output points to be modelled after spatial truncation has been applied. The error message for no output points remaining within the truncation region is shown in **Figure 6.5**.

When the ADMS-Urban RML system is run with the **Output type** set to **Receptor locations**, the initial check runs (described in Step 2 of Section 8.2) run ADMS-Urban with spatial truncation to each regional model grid cell within the nesting domain. A regional model grid cell which contains no output points will be excluded from further processing by the RML Controller. The ADMS-Urban RML system run containing excluded cells is likely to complete successfully, provided at least one cell is included in the run.

When the ADMS-Urban RML system is run with the **Output type** set to **Grid for contouring**, the initial check runs are not performed. The **Create ASP** run (described in Section 8.3.1) will fail if there is no overlap between the nesting domain and the output points defined in the .upl with explicit sources. If one or more grid cells within

a larger nesting domain do not contain any output points, these cells will fail at the main ADMS-Urban runs. The ADMS-Urban RML system run containing failed cells is likely to fail at the **AddInterpIGP** utility stage, as gridded output locations are required to form a complete rectangular grid.

Solution: Check that the nesting domain and all output point locations in the input .upl files are defined in the same coordinate system.

6.5 Run Manager

In general, Run Manager will not issue error messages to the user when used as part of the ADMS-Urban RML system. During a complete run of the ADMS-Urban RML system, the user should only use the Run Manager interface to view progress of ADMS-Urban model runs, while the RML Controller will perform all the required tasks for initialising, collecting and deleting runs, as described in Section 8.5.2.1. However, if a run of the ADMS-Urban RML system is interrupted, it may be necessary for the user to delete some failed or unwanted runs using the Run Manager interface, as described in Section 6.5.1 below.

6.5.1 Deleting failed or unwanted runs

Problem: The usual processes which collect and delete ADMS-Urban model runs from Run Manager may be interrupted if either the machine running the RML Controller or the machine on which the Run Manager central repository is located experience a failure during an ADMS-Urban RML system run, or there is a network failure which prevents the RML Controller machine communicating with the central repository. In this case, or in some circumstances when the user cancels an ADMS-Urban RML system run, some ADMS-Urban model runs or run files may be left on the runs machines.

Solution: Open the Run Status screen in Run Manager to view all current model runs. Indications of failed runs include:

- blank **Progress** and **Predicted End** entries for a run in the **Executing** section of the **Run Status** screen with a **Start Time** entry more than a few minutes earlier;
- a red **Progress** bar for a run in the **Executing** section of the **Run Status** screen;
- runs appearing in the **Failed** section of the **Run Status** screen.

Use the kill or delete buttons to stop failed or unwanted runs and remove their files from the runs machine.

6.6 WRFtoMet utility

Errors from the **WRFtoMet** utility are written to a .txt file, in the same directory as the relevant input text file. The **WRFtoMet** utility is run separately for each regional model grid cell within the nesting domain. Hence any error files from the utility are stored in directories for each grid cell, as described in Section 5.1.3.

6.6.1 Could not open WRF output file

```
WarningWRFToMet13500_-674000.txt - Notepad

File Edit Format View Help

C:\Program Files\CERC\RML\WRFtoMet.exe

Problem: Could not open WRF file, it may not exist: P:\WRF\201003\wrfout_d04_2010-03-31_170000

Date/time: 18/9/2014 13:24:56
Input directory: "C:\Program Files\CERC\RML"
Output file: "C:\Program Files\CERC\RML\Working\13500_-674000\13500_-674000MetData.met"

Version: 1
```

Figure 6.6 Error message if WRFtoMet cannot open a WRF output file

The error message issued if the **WRFtoMet** utility could not open a WRF output file is shown in **Figure 6.6**. There are two possible causes for this error, which are described below with suggested solutions.

Problem 1: This error may indicate an inaccuracy in the file directory and/or file name template specification for the WRF output files, if the file path quoted in the error message is incorrect.

Solution 1: Check the meteorological model file directory and file name template specified in the ADMS-Urban RML Controller interface, as described in Sections 4.3.2.1 and 4.3.2.2.

Problem 2: If the file path quoted in the error message is correct, there may be a problem with the utility accessing the file.

Solution 2: Check that:

- the access permissions for the directories containing the data files are set appropriately;
- any network connection between the RML Controller machine and the directory containing the data files is operating correctly; and
- the files are not simultaneously being used by any other user or process.

6.6.2 Error extracting variable from WRF

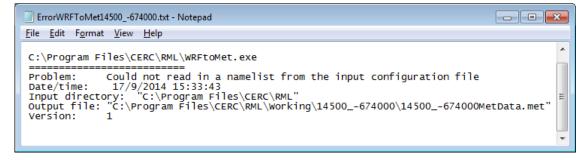


Figure 6.7 Error message if a specified variable name is not available in the WRF output files

Problem: **Figure 6.7** shows an example of the error message which will be issued if a variable cannot be found in the WRF output files. This may indicate an error in the **WRFtoMet** input text file, such that the variable name specified in the input text file

does not correspond to a variable name in the WRF output file.

Solution: Check that the variable names being used in the **WRFtoMet** input text file correspond to netCDF variable names in the WRF output file(s).

6.7 RML Background utility

Errors and warnings from the **RML Background** utility are written to *.txt* files, in the same directory as the relevant input text file. The **RML Background** utility is run separately for each regional model grid cell within the nesting domain. Hence any error files from the utility are stored in directories for each grid cell, as described in Section 5.1.3.

6.7.1 Regional model output file does not exist

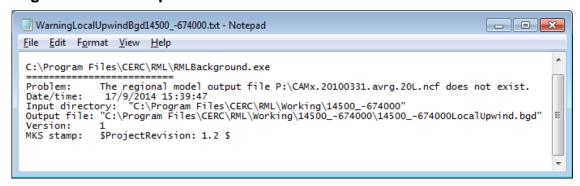


Figure 6.8 Error message if a specified regional model concentration output file does not exist

The error message issued if the **RML Background** utility could not open a regional model concentration output file is shown in **Figure 6.8**. There are two possible causes for this error, which are described below with suggested solutions.

Problem 1: This error may indicate an inaccuracy in the file directory and/or file name template for the regional model concentration output files, if the file path quoted in the error message is incorrect.

Solution 1: Check the file directory and file name template specified for the regional concentration model output files in the ADMS-Urban RML Controller interface, as described in Sections 4.3.3.2 and 4.3.3.3.

Problem 2: If the file path quoted in the error message is correct, the utility may not be able to access the relevant file.

Solution 2: Check the access permissions for the directories containing the regional model output data and any network connection between the RML Controller machine and the data storage directory.

6.7.2 Specified regional model output file not opened correctly

Problem: An error message that a specified regional model output file has not been

opened correctly indicates that the utility cannot access the relevant file.

Solution: Check any network connection between the RML Controller machine and the data storage directory and that the files are not simultaneously being used by any other user or process.

6.7.3 Error in netCDF function

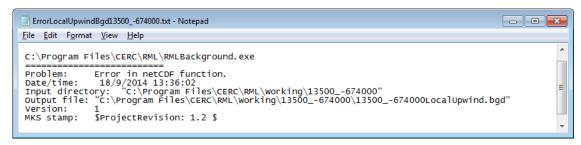


Figure 6.9 Error message for a problem with the regional model concentration output file format

Figure 6.9 shows the 'Error in netCDF function' message which may indicate various problems, as described below.

Problem 1: The regional model concentration output files may not be in the expected format, such that the utility cannot find grid definition or time variables.

Solution 1: Check that the files are in the correct format for the relevant regional model, for example by using a compatible data viewer.

Problem 2: One or more of the regional model species names given in the species map file may not be a valid variable name for the concentration output files.

Solution 2: Check that the names used in the species map file exactly match the species variable names in the regional model concentration output files.

6.7.4 Error in reading input text file

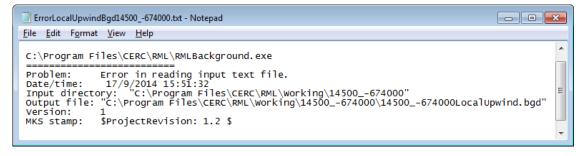


Figure 6.10 Error message for a problem with the species map file contents

Problem: An "Error in reading input text file" message, as shown in **Figure 6.10**, will be issued if the species map file is not in the correct format.

Solution: Check that the species map file format matches the definition given in

Section 4.3.3.6.

6.7.5 Nesting domain boundary not aligned with regional model cell boundary

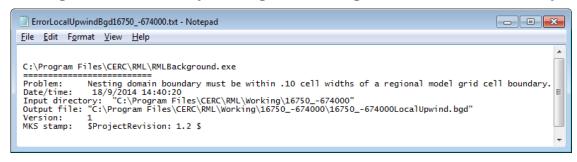


Figure 6.11 Error message issued if the nesting domain boundaries do not align with regional model grid cell boundaries

Problem: The RML Background utility requires the input nesting domain extents to be aligned with regional model grid cell boundaries to within 0.1 of the cell spacing. If this is not the case, the error message shown in **Figure 6.11** will be issued.

Solution: Check that the boundaries of the nesting domain you have defined align with regional model grid cell boundaries and that the regional model grid definition is correct.

6.7.6 Negative nesting background (nesting mode only)

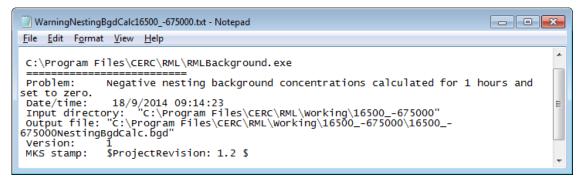


Figure 6.12 Warning message about the number of hours when negative nesting background concentrations were calculated

Problem: Nesting background concentrations are calculated as a difference between regional model concentrations and ADMS-Urban concentrations excluding background from the .upl with gridded emissions matching those used in the regional model. If the ADMS-Urban concentration is larger than the regional model concentration, a negative nesting background concentration can be calculated. The RML Background utility will set negative nesting background concentrations to zero in the output background file, but will output a warning with the total number of hours where a negative concentration was calculated for any pollutant, as shown in Figure 6.12. Negative values for a small proportion of modelled hours, which may be of very small magnitude, can be caused by minor differences in dispersion calculations between ADMS-Urban and the regional dispersion model and may be ignored.

Negative nesting background concentrations calculated for a substantial proportion of the modelled hours, for example more than 5%, indicate inconsistencies between the ADMS-Urban model set-up for the *.upl* with gridded emissions for nesting background and the regional model.

Solution: Check that:

- the horizontal grid definition for the ADMS-Urban grid source cells and the regional model grid cells is consistent;
- the ADMS-Urban grid source depth is twice the height of the lowest regional model grid layer;
- there is one output point defined in the centre of each ADMS-Urban grid source cell;
- the total magnitude of emissions from each ADMS-Urban grid source cell is the same as that from the corresponding regional model cell; and
- the time-variation of emissions from the ADMS-Urban grid source corresponds as closely as possible to the time-variation of emissions from the regional model within the nesting domain.

Analysis of the diurnal profiles of:

- regional model concentrations;
- local upwind background concentrations;
- ADMS-Urban concentrations output from the .upl with gridded emissions for nesting background; and
- nesting background concentrations

may assist with identifying inconsistencies with the magnitude and/or time-variation of emissions used in ADMS-Urban and in the regional model.

6.7.7 ADMS species not found (nesting mode only)

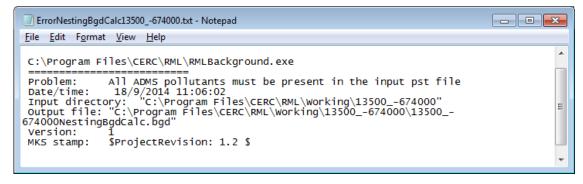


Figure 6.13 Error message if any ADMS species have not been found in the input .pst file

Problem: **Figure 6.13** shows the error message that will be issued by the RML Background utility if any ADMS species were not found in the input .pst file. This may indicate that the species map list of ADMS species does not match the species names used in the ADMS-Urban .upls, or that not all the ADMS species listed in the

species map have been included as output from the .upl with gridded emissions for nesting background.

Solution: Check that the ADMS species names in the species map file match those used in the .upls and that all ADMS species from the species map file are defined as outputs with one hour averaging time from the .upl with gridded emissions for nesting background, as described in Section 4.4.1.1.

6.8 RML Output utility

Errors and warnings from the **RML Output** utility are written to .txt files, in the same directory as the relevant input text file. The **RML Output** utility is run separately for each regional model grid cell within the nesting domain. Hence any error files from the utility are stored in directories for each grid cell, as described in Section 5.1.3.

6.8.1 Regional model output file does not exist

Figure 6.14 An example error message for a problem accessing regional model concentration output files

Problem: If the RML Background utility has run successfully, the file directory and file name template specified in the ADMS-Urban RML Controller interface for the regional model output concentration files must be correct. Hence an error message from the RML Output utility that a regional model output file does not exist, as shown in Figure 6.14, indicates a problem with accessing the relevant file.

Solution: Check any network connection between the RML Controller machine and the data storage directory and the permissions set for the data storage directory.

6.8.2 Specified regional model output file not opened correctly

Problem: An error message that a specified regional model output file has not been opened correctly indicates that the utility cannot access the relevant file.

Solution: Check that:

• any network connection between the RML Controller machine and the data storage directory is functioning correctly;

- the permissions for the data storage directory are set so the RML Controller machine can read the files; and
- the files are not simultaneously being used by any other user or process.

6.8.3 ADMS species not found

```
ErrorRMLOutput16500_-674000.txt - Notepad

File Edit Format View Help

C:\Program Files\CERC\RML\RMLOutput.exe

Problem: Not all ADMS pollutants defined in the species map file have been found in ADMS output file number 1 as concentration datasets with 1-hour averaging time.

Date/time: 18/9/2014 11:22:44
Input directory: "C:\Program Files\CERC\RML\working\16500_-674000"
Output file: "C:\Program Files\CERC\RML\working\16500_-674000\"
Output file: "C:\Program Files\CERC\RML\working\16500_-674000\"
Oversion: 1
MKS stamp: $ProjectRevision: 1.2 $
```

Figure 6.15 Error message if some ADMS species have not been found in the ADMS-Urban output files

Problem: **Figure 6.15** shows the error message that will be issued if ADMS species have not been found in the ADMS-Urban output files. This may indicate that the species map list of ADMS species does not match the species names used in the ADMS-Urban .upls, or that not all the ADMS species listed in the species map have been included as output from the .upls for the main nesting ADMS-Urban runs.

Solution: Check that the ADMS species names in the species map file match those used in the *.upls* and that all ADMS species from the species map file are defined as outputs with one hour averaging time from both of the *.upls* for the main nesting ADMS-Urban runs, as described in Sections 4.4.1.2 and 4.4.1.3.

SECTION 7 Worked examples

In this section, worked examples to guide you through setting up some basic ADMS-Urban RML system runs and presenting their results are described. It is recommended that you work through these examples when starting to use the ADMS-Urban RML system. Note that a complete set of the resulting ADMS-Urban RML system input and output files can be found in the *<install_path>\Examples* directory.

Section X gives a brief description of the example regional model data files which are supplied with the ADMS-Urban RML Controller installation.

The examples cover the use of the ADMS Comprehensive Output File Processor utility with output from the ADMS-Urban RML system. Further details regarding the ADMS Comprehensive Output File Processor can be found in the ADMS Comprehensive Output File Processor User Guide, which can be found in the ADMS-Urban RML <install_path>\Documents\ directory.

The second example covers the use of ADMS-Urban RML system output in the ADMS Mapper. Further details regarding using the ADMS Mapper can be found in the ADMS Mapper User Guide which can be accessed from the **Help** menu of the ADMS Mapper.

You can launch the ADMS-Urban RML Controller interface in several different ways:

- double-click on the icon for the shortcut created during installation (refer to Section 2.2.2 for details);
- use the Windows Start menu and select Programs, ADMS-Urban RML; or
- go to the main ADMS-Urban RML Controller directory *<install_path>* and double-click on the file *Quad.exe*.

It is strongly recommended to create an additional directory for setting up and running these examples, in order to keep them separate from the examples provided in <install_path>\Examples directory supplied with the model.

Please note that Run Manager must be set up to run ADMS-Urban before the worked examples can be attempted. Refer to the Run Manager User Guide for information on how to do this.

7.1 Example regional model data

The example regional model data files which are supplied as part of the ADMS-Urban RML Controller installation consist of 72 WRF output files, each containing one hour of data, and three CAMx output files, each containing 24 hours of data. Although the models were originally run with larger modelling domains, the supplied data has been extracted to cover a rectangular area of 4 x 5 cells. The grid resolution is 1 km in each direction. The number of chemical species contained in the CAMx output files has also been reduced compared to the

internal model speciation.

The time period covered by the regional model data files is midnight on 3rd March 2010 to 11 pm on 5th March 2010 in UTC. There is a time difference of eight hours between local solar time and UTC, so the time period in local time is 8 am on 3rd March 2010 to 7 am on 6th March 2010. Concentrations of NO₂ from the CAMx output file for 6 pm on 3rd March 2010 in UTC are shown in **Figure 7.1**, as displayed in the free VERDI visualisation software (Adams and Del Vecchio, 2013).

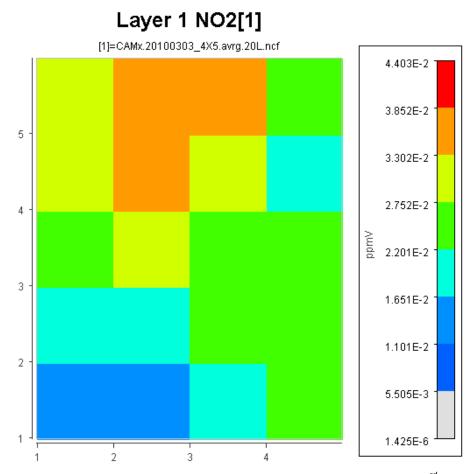


Figure 7.1 Plot of example CAMx ground-level NO₂ concentrations in ppmV for 3rd March 2010 at 18:00 UTC (4th March 2010 at 00:00 local time), visualised in VERDI.

7.2 Example 1: Modelling with output at receptor locations

In this example you will carry out a simple ADMS-Urban RML system run, with output at receptor locations, as may be used for model validation.

7.2.1 Setting up the run

Step 1 Start by ensuring that the ADMS-Urban input files are set up properly. First check the background .upl. Start ADMS-Urban, click on File, Open and browse to the file called Background.upl in the <install_path>\Examples directory. This file contains the source emissions equivalent to those in the regional model.

- Step 2 This .upl file is already set up. Look through each of the tabs to check the inputs the only sources present are grid sources and there is a specified point located in the centre of each of the grid cells. From the Utilities menu, select ADMS Mapper to launch the ADMS Mapper and view these sources and output points.
- **Step 3** If you have not already made a local working copy of this file, make one now by clicking **File**, **Save As** and browsing to your local working directory. It is not recommended that files are saved in the installation directory.
- Step 4 Repeat Steps 1-3 with the file *Explicit.upl* from the <*install_path*>*Examples* directory. Viewing this .*upl* file in the ADMS Mapper will display the explicit ADMS-Urban sources that are present within the ADMS-Urban modelling area, and the receptor points at which concentration output will be obtained, as shown in **Figure 7.2**.

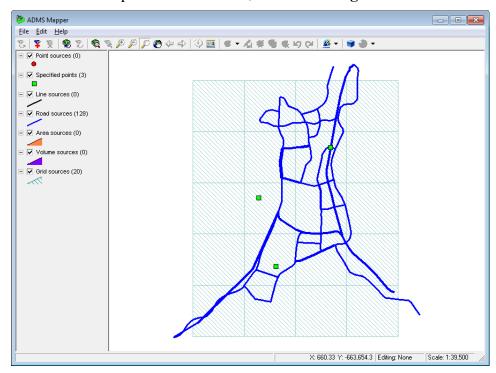


Figure 7.2 The explicitly modelled sources and receptor locations in Example 1.

- Step 5 Once a local working copy of *Explicit.upl* has been created, the file with equivalent gridded emissions must be created. Create another working copy of *Explicit.upl* and name it *Gridded.upl*.
- Step 6 All of the explicit sources must now be deleted from *Gridded.upl*. In the Source tab in ADMS-Urban, select to show **Road Sources** and then click **Delete all**. In this example, there are no explicit industrial sources defined, in general these would also need to be deleted.
- Step 7 Now that the ADMS-Urban run files have been set up, the RML input parameters can be defined. Close ADMS-Urban and start the ADMS-Urban RML.

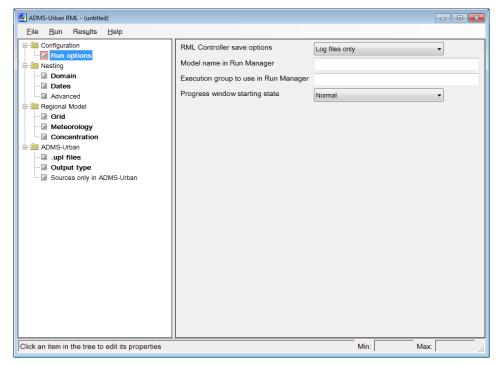


Figure 7.3 The ADMS-Urban RML Controller interface.

- Step 8 From the RML Controller save options, select All files from the list. Enter the model name that you have given ADMS-Urban in Run Manager and the name of the execution group that you would like to carry out the nesting runs. Be aware that the Run Manager names are case sensitive.
- Step 9 Click on the **Nesting**, **Domain** section in the tree view on the left side of the screen. This is where the extent of the nested area is defined, which must cover the grid cells that contain the output points. Set the centre of the nesting domain to be (-3000, -664000) and the extents to be (2000, 3000).
- **Step 10** Next, navigate to the **Nesting, Dates** section. Here, select the start and end dates to cover the full extent covered by the regional model files. Set the start date to be 03 March 2010 at 09:00 and the end date to be 06 March 2010 at 07:00.
- Step 11 The Regional Model inputs now need to be defined, these should reflect the data contained in the regional model output files. In the Grid section, set the Coordinates of the bottom left corner of the grid to be (-5000, -666500), the Grid spacings to be (1000, 1000) and the Number of grid cells in each direction to be (4, 5).
- Step 12 The Meteorology section is where the regional meteorology files must be defined. Set the directory that contains the WRF meteorology files, for example <install_path>\Data\WRF, and set the naming pattern for the WRF files as wrfout_d04_%Y-%M-%D_%h_%m_%s. The Number of hours contained in each meteorological data file should be set to 1 and the Time difference between local time and the meteorological data is 8 hours. You do not need to specify a custom WRFtoMet file for this example.
- Step 13 The Concentration section is where the regional model used to model concentration is defined. In this example, CAMx files are being used. Enter the directory that contains the CAMx files, for example

<install_path>\Data\CAMx, and set the naming pattern for the CAMx files as CAMx.%Y%M%D_4X5.avrg.20L.ncf. There are 24 hours of data in each CAMx file and the time difference is 8 hours. Enter the path of the provided species map file, for example <install_path>\Data\ADMS_CAMx_SpeciesMap.csv. The Reference sealevel temperature should be set to 25°C. Tick to Specify reference pressure for the top of the model and set it to be 5000 Pa.

Step 14 In the **ADMS-Urban**, .upl files section, enter the full path to the working copies of your background .upl, gridded nesting .upl and explicit nesting .upl in the boxes. Click the folder buttons to the right of the boxes to browse to the files.

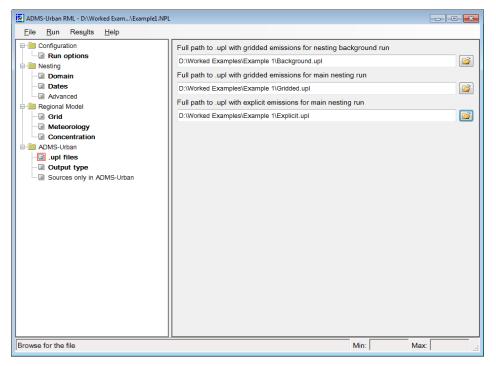


Figure 7.4 The ADMS-Urban RML .upl files screen.

- Step 15 In the Output Type section, select Receptor locations as the ADMS-Urban output type.
- **Step 16** Save the RML input parameters in an .npl file by clicking **File**, **Save As...**, then enter the filename *Example1.npl* and browse to the directory where you would like to save the file. Click **OK** to save the file.

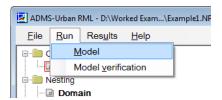


Figure 7.5 The ADMS-Urban RML Run menu.

Step 17 To carry out the nesting run, select Run, Model from the menus, as shown in Figure 7.5.

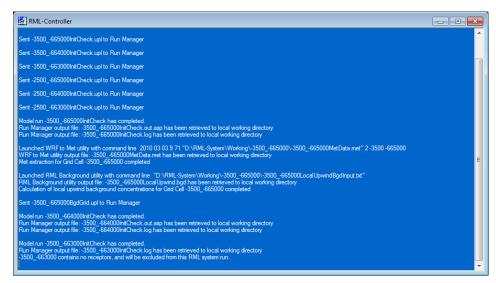


Figure 7.6 The ADMS-Urban RML Controller progress window.

Once the nesting run has completed, the RML Controller progress window will display a summary of the RML system run, as shown in **Figure 7.6**. Despite the nesting domain consisting of six regional model cells, only three of them will have been run as only three of the cells contain output points. The cells which do not contain output points are excluded from the run. You will also notice that a new folder called *Example1 - other files* has been created in the directory where the *.npl* was saved. This will contain all of the files created during the run. As you selected to keep **All files**, this folder will contain a large number of files, including input, intermediate and output files for each grid cell.

7.2.2 Extracting data to a text file

The following steps describe how to extract the concentration data from the netCDF Comprehensive Output file that is output from the ADMS-Urban RML system to create an ADMS-Urban format text file. Once you have created this text file you can process the data in the same way that you would process the output from an ordinary ADMS-Urban model run.

- Step 1 Once the run has finished, choose Extract statistics... from the Results menu to open the Comprehensive Output File Processor (COFP).
- Step 2 The output file from the RML system run will automatically be loaded into the COFP if the related .npl is loaded into the RML interface. If it is not automatically loaded, then click **Browse...** and browse to locate your comprehensive output file.
- Step 3 Click Create Output to open the Create Output Files screen, as shown in Figure 7.7.

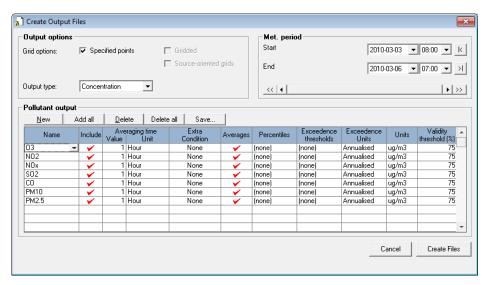


Figure 7.7 The COFP Create Output Files screen.

- Step 4 We want to create files containing specified point concentrations over the whole of the modelled time period, so the default **Output options** and **Met.** period do not need to be changed. In the **Pollutant output** section, click **Add all** to add a row in the **Pollutant output** table for each of the modelled pollutants. Change the **Averaging time Unit** from **Period** to **Hour** for all pollutants.
- Step 5 Click **Create Files**, browse to a suitable location, give the file the filename *Example1* and then click **Save** to begin extracting the data to a *.pst* text file. Be aware that any existing files of the same name will be overwritten automatically. After the output file has been created, click **Yes** to view it in Explorer.

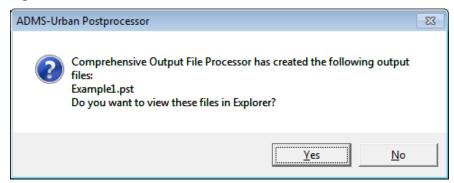


Figure 7.8 The message that is displayed after the COFP has created the output files.

Please refer to the Comprehensive Output File Processor User Guide for more information on using the COFP.

7.2.3 Analysing data

The .pst file output from the COFP is a standard ADMS-Urban format, which is a comma-separated text file so it can be easily analysed using Excel, for example to create a time series graph.

- Step 1 Start Microsoft Excel.
- Step 2 Click File and select Open.

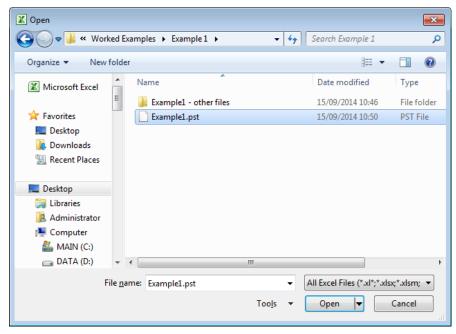


Figure 7.9 Opening a *.pst file in Excel.

- Step 3 Type '*.pst' in the **File name:** box and press **Enter** to display all of the ADMS-Urban specified points output files. Select the file *Example1.pst* that you have just created and click **Open**. This launches the **Text Import Wizard**.
- Step 4 In the Original data type box, choose the Delimited option and click Next > to move on to the next section of the Wizard.

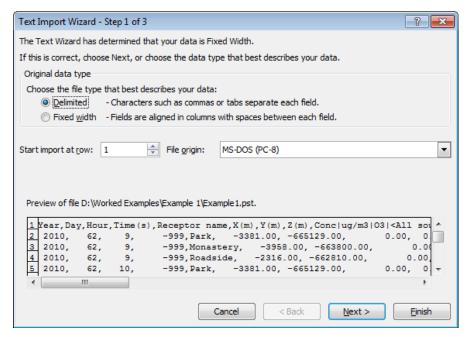


Figure 7.10 Microsoft Excel Text Import Wizard - Step 1 of 3.

Step 5 In the **Delimiters** box, select the **Comma** check box and then click **Next >** to move onto the final step of the Wizard.

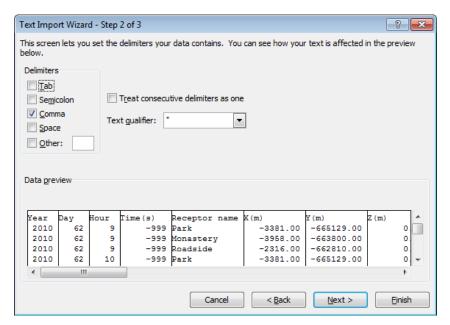


Figure 7.11 Microsoft Excel Text Import Wizard - Step 2 of 3

- Step 6 Ensure that the file has been properly separated in the **Data preview** box, and click the **Finish** button to import the data.
- Step 7 To filter the data by receptor column (in this case column E), highlight the appropriate column header and then, from the **Sort & Filter** section of the **Data** ribbon, select **Filter**. Click the arrow in the receptor column and choose one of the receptor names from the list.

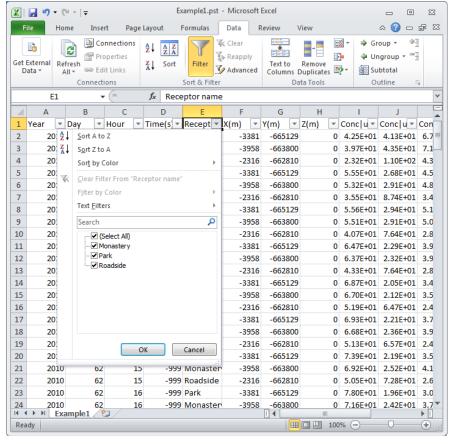


Figure 7.12 Filtering the data.

Step 8 Next, highlight the hour column and the concentration column that you would like to plot.

Hold down the Ctrl key to select non-adjacent columns.

Step 9 To create a time series chart of concentrations, from the **Charts** section of the **Insert** ribbon, choose a **Scatter** chart with lines. Click on the chart that has just been created and, in the **Location** section of the **Chart Tools**, **Design** ribbon, select **Move Chart**, and then select the **New Sheet** option.

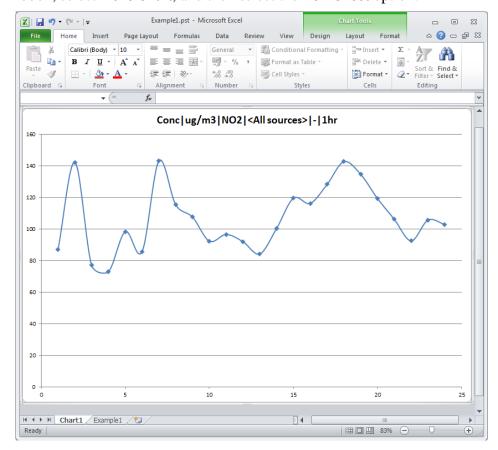


Figure 7.13 Time series graph.

If this run had been carried out for the purpose of model validation, then the MyAir toolkit can be used to create graphs and statistics comparing the modelled concentrations to observed values. For more information, please refer to the MyAir Model Evaluation Toolkit User Guide (CERC, 2013b).

7.3 Example 2: Modelling with gridded output for contours

7.3.1 Setting up the run

- Step 1 Make a copy of all three .upl files that were used in Example 1, and put them in a new working directory. Rename the files Background2.upl, Explicit2.upl and Gridded2.upl.
- **Step 2** Open *Explicit2.upl* in ADMS-Urban.

- Step 3 In the **Grids** tab, select **Gridded** output. The output grid has already been defined it covers the central six regional model grid cells.
- Step 4 Tick to include Road, Line Source-oriented grids.

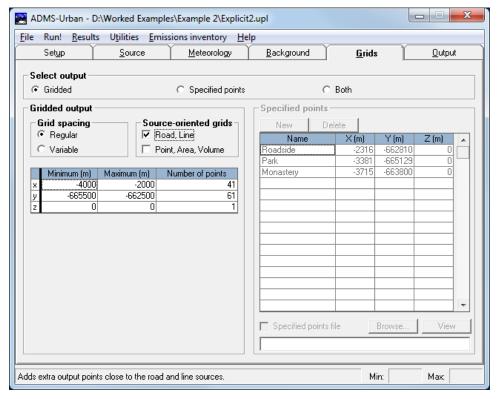


Figure 7.14 ADMS-Urban Grids screen with Road, Line Source-oriented grids selected.

- **Step 5** Start the ADMS Mapper to view the output grid and sources.
- **Step 6** Save *Explicit2.upl* and close ADMS-Urban.

Background2.upl and Gridded2.upl do not need to be changed for this example.

- **Step 7** Instead of creating a new .npl file from scratch, make a copy of Example1.npl and name it Example2.npl.
- **Step 8** Start the ADMS-Urban RML and open *Example2.npl*.
- Step 9 We do not need to keep all of the run files this time, so in the **Run options** section, select to save only the **Key files**.
- **Step 10** The only other inputs that are different than those used in Example 1 are those in the **ADMS-Urban** section. In the .upl files screen, change the paths of the three .upl files to use Background2.upl, Gridded2.upl and Explicit2.upl.

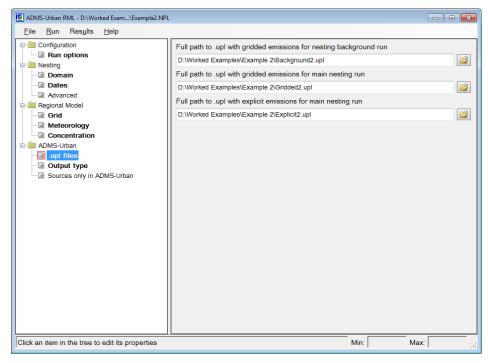


Figure 7.15 ADMS-Urban RML .upl files screen.

- Step 11 In the Output type section, change the ADMS-Urban output type to be Grid for contouring.
- **Step 12** Save *Example 2.npl* and then run the model. This will take longer than Example 1 as there are a greater number of output points and calculations will be performed for all six regional model grid cells.

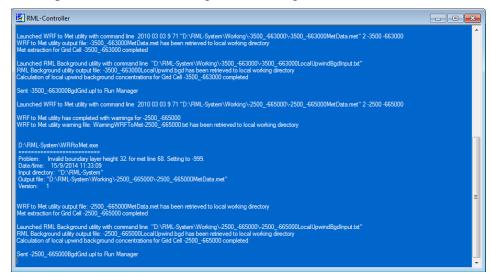


Figure 7.16 ADMS-Urban RML Controller progress window

7.3.2 Extracting statistics to a text file

- **Step 1** Start the COFP and make sure the file *Example2.nc* is loaded.
- Step 2 Click Create Output.

Step 3 We want to create files containing grid concentrations for contouring over the whole of the modelled time period, so the default **Output options** and the **Met. period** do not need to be changed. In the **Pollutant output** section, click **Add all** to add a row in the **Pollutant output** table for each of the modelled pollutants. This time, we will be creating contours of the average concentration over the whole modelled period so you do not need to change the **Averaging time Unit** from its default value.

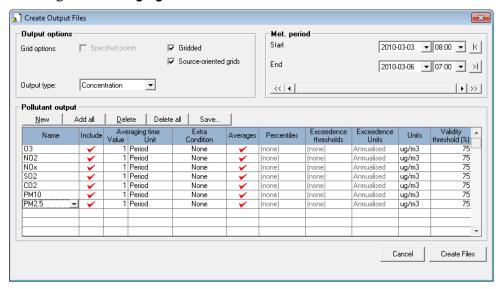


Figure 7.17 The COFP Create Output Files screen.

Step 4 Click Create Files, browse to a suitable location, give the file the filename *Example2* and then click Save to begin extracting the data to a *.glt* text file. Be aware that any existing files of the same name will be overwritten automatically. After the output file has been created, click Yes to view it in Explorer.

7.3.3 Plotting contours of concentration

The instructions given in this worked example demonstrate how to create contour plots in the ADMS Mapper. It is also possible to create contour plots in third party visualisation software, please refer to the ADMS-Urban GIS link user guides for details of how to do this.

- Step 1 Start ADMS-Urban, then from the **Utilities** menu, select **ADMS Mapper**.
- Step 2 In the ADMS Mapper, click the **Contour** icon on the toolbar to open the ADMS Contour Plotter.
- **Step 3** Select the **Long term** option.
- **Step 4** In the left hand pane, browse to the working directory for Example 2 and select the .*glt* file that you have just created.
- **Step 5** In the right hand pane, select NO_2 as the **Dataset to plot**.

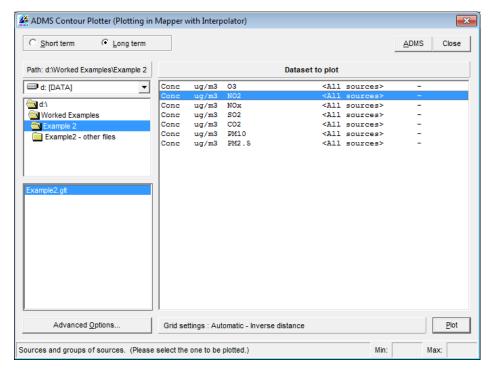


Figure 7.18 The ADMS Contour Plotter.

- Step 6 Click Advanced Options... and select Inverse distance from the Gridding method list. Click Close to exit the Advanced Contour Options screen.
- Step 7 Click **Plot** and browse to a location to save the contour grid. Give the grid file a suitable name and click **Save** to create the contour plot in the ADMS Mapper. Please refer to the ADMS Mapper User Guide for details of how to change the appearance of the contour plot.

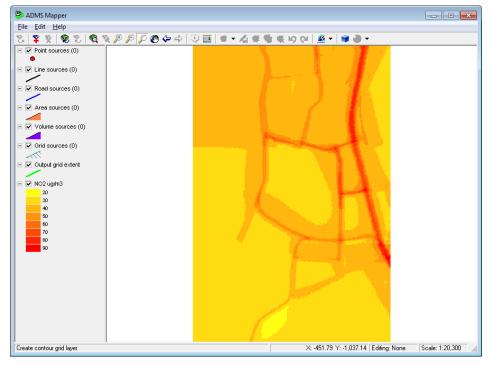


Figure 7.19 Contour plot of NO₂ being displayed in the ADMS Mapper.

7.4 Example 3: Modelling a new development

In this example you will be modelling a planned new development, where the main sources of emissions will be a boiler stack and a road leading to the development. The proposed location of the new buildings is slightly to the south of the Monastery receptor location. New emissions only need to be added to the *.upl* file with explicity emissions, as explained in Section 4.4.3, because the new sources will only be present in ADMS-Urban and not in the regional model.

7.4.1 Setting up the run

- Step 1 Create a new working directory for Example 3 and copy *Background2.upl*, *Explicit2.upl*, *Gridded2.upl* and *Example2.npl* from the Example 2 working directory to the new directory. Renumber all of the copied files from 2 to 3 (e.g. change *Example2.npl* to *Example3.npl*).
- **Step 2** Start ADMS-Urban and open *Explicit3.upl*.
- **Step 3** On the **Grids** tab, choose **Both** as the selected output.
- **Step 4** Open the ADMS Mapper.
- Step 5 The new development is going to be located near the Monastery receptor, so using the **Zoom** tool, zoom in to that area, as shown in **Figure 7.20**.

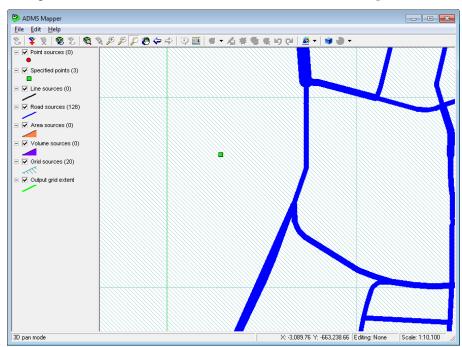


Figure 7.20 Zoomed in to the area of the new development.

- **Step 6** The new boiler stack will be modelled as a point source. In the left hand pane, click on **Point sources**, this allows us to add new point sources.
- Step 7 To add a new point source, click on the Add feature button in the toolbar at the top of the screen, as shown in Figure 7.21.

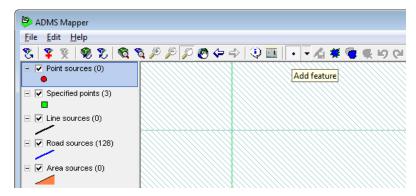


Figure 7.21 Selecting the Add feature tool for Point sources.

Step 8 Click the screen at the point where you would like to add the new point source, place it slightly to the south of the Monastery receptor point as shown in **Figure 7.22**. Upon clicking to create the new point source, the ADMS-Urban interface will become active and the **Industrial sources** section of the **Source** tab will display the newly created point source.

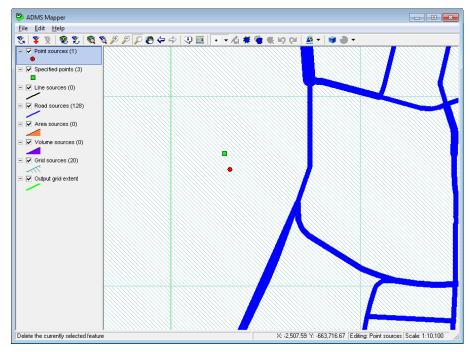


Figure 7.22 The newly added point source.

Step 9 You now need to enter the source parameters for the new point source. Change the Name of the source to be "Boiler". Set the Height to 25 m, the Diam. (stack diameter) to be 0.5 m, the Vel (exit velocity) to 8 m/s and the Temp. (stack exit temperature) to 180°C.

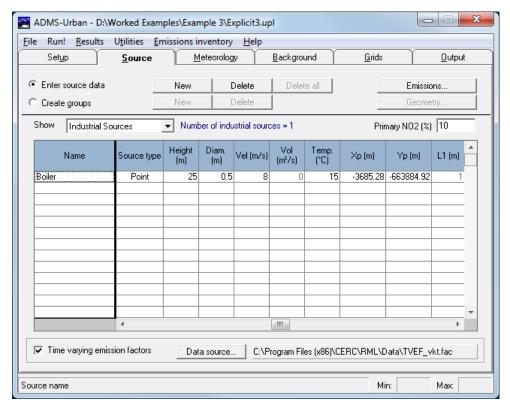


Figure 7.23 The new point source with stack parameters defined.

- **Step 10** Click the **Emissions...** button to open the Emissions screen.
- **Step 11** By default, the pollutant NO_x will be displayed. Click **New** three times and change the three new pollutants to be CO, PM_{10} and $PM_{2.5}$.
- **Step 12** Change the emission rates to be 0.7 g/s for NO_x , 0.15 g/s for CO, 0.05 g/s for PM_{10} and 0.03 g/s for $PM_{2.5}$. Click **OK** to close the Emissions screen.

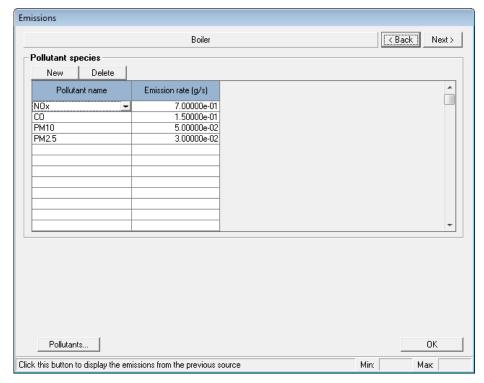


Figure 7.24 The emission rates for the Boiler.

- Step 13 NO_2 emissions will be defined as a percentage of the NO_x emissions. Keep the **Primary NO2 (%)** as 10%.
- **Step 14** Next, switch back to the ADMS Mapper and highlight **Road sources** in the left-hand pane.
- **Step 15** Select the **Add feature** button \(\strice{\cdot} \).

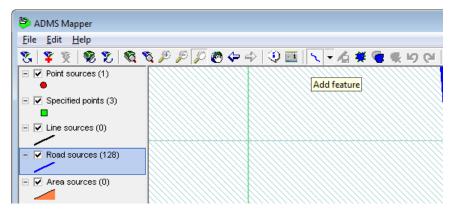


Figure 7.25 The Add feature button for Road sources.

Step 16 Click on the location for the first road vertex at the point where the existing road bends, to the east of the Monastery receptor. The proposed route for the new road starts at the existing road and ends just past the new boiler, with the road passing between the Boiler and the Monastery, as shown in **Figure 7.26**. Double click at the final vertex to complete the road.

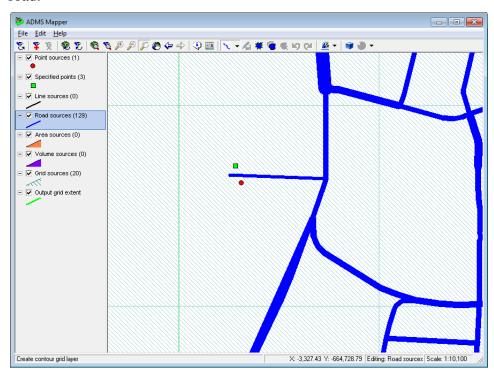


Figure 7.26 The newly defined road.

Step 17 The ADMS-Urban interface will then be activated, displaying your new road source in the **Source** tab. Change the road **Name** to be "Access road" and the **Road width** to be 11 m.

- Step 18 Click Emissions... and select the All pollutants user defined option.
- **Step 19** Click **New** until there are six pollutants defined and make sure these pollutants are NO_x, PM₁₀, PM_{2.5}, CO, VOC and NO₂. Set the emission rates to: NO_x 0.1 g/km/s, PM₁₀ 0.005 g/km/s, PM_{2.5} 0.003 g/km/s, CO 0.06 g/km/s, VOC 0.005 g/km/s and NO₂ 0.02 g/km/s.

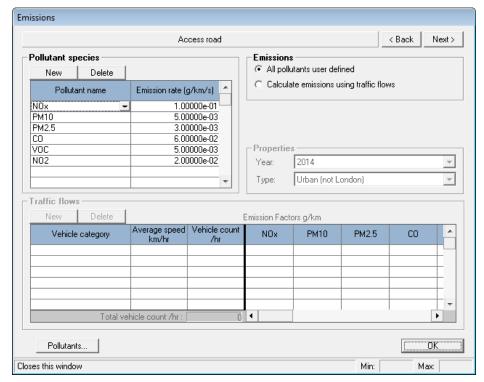


Figure 7.27 The pollutant emission rates for the new Access road.

Step 20 The newly added emissions now also need to be added into the grid source. To do this, the individual source emissions must be averaged over the whole grid cell. You will need to add the contribution of the two new sources to the current grid cell emissions in cell #-004000_-664500. The easiest method of doing this is to calculate the grid-averaged emission rates for each pollutant for each new source and then add them onto the current grid emission rates in a spreadsheet, as shown in Figure 7.28, before overwriting the grid cell emission rates in ADMS-Urban.

For the new point source, simply divide the emission rate in g/s for each pollutant by the area of the grid cell in m^2 (1,000,000 m^2), and then add this onto the current emission rate for the grid cell. For example, the emission rate to add on for NO_x would be: $0.7 / 1x10^6 = 7x10^{-7}$ g/m²/s. Remember to do this for NO_2 as well, by taking 10% of the NO_x value.

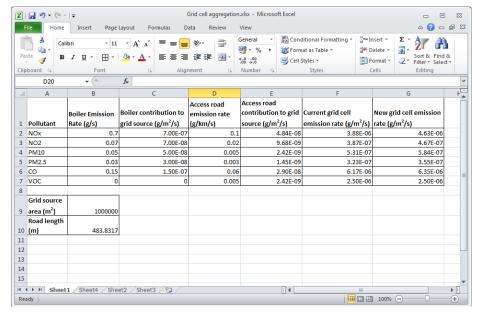


Figure 7.28 Calculating the new grid source emissions.

Step 21 Adding the new road source contribution to the grid cell emissions requires you to know the length of the road you have just created. This can be found using the ADMS Mapper, by selecting the Information tool then clicking the Access road. The length is given by the GIS_LENGTH attribute.

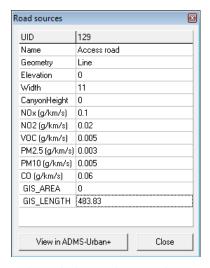


Figure 7.29 The information relating to the new Access road from the ADMS Mapper, with the road length highlighted.

Step 22 The emission rates of the road source, which are given in g/km/s, must be converted into the units required for inclusion in the grid cell, g/m²/s. To do this, multiply the emission rate for each pollutant by the length of the road in km, to obtain an emission rate in g/s, then divide those emission rates by the area of the grid cell in m² (1,000,000 m²). Finally, add these emission rates onto the current grid cell totals.

For example, for a road that is 500 m long, the emission rate to add on for NO_x would be: $0.1 \times 0.5 / 1 \times 10^6 = 5 \times 10^{-8} \text{ g/m}^2/\text{s}$. The grid-averaged emission rate for your road will be slightly different to this, depending on its length.

Step 23 Use the ADMS-Urban interface to navigate to the **Emissions** screen for the grid source cell #-004000_-664500, as shown in **Figure 7.30**. Enter the modified emission rates including the effects of the new sources, as calculated in the spreadsheet.

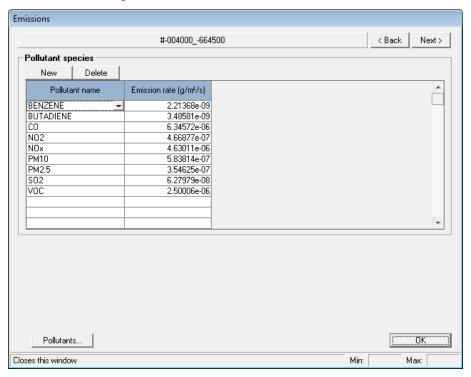


Figure 7.30 Grid source cell #-004000_-664500 with the emission contributions from the new sources included.

- **Step 24** Save *Explicit3.upl*, and then close the ADMS Mapper and ADMS-Urban.
- **Step 25** Start the ADMS-Urban RML and open *Example3.npl*.
- Step 26 Change the Run options to keep Log files only.
- Step 27 Change the .upl files to use Background3.upl, Gridded3.upl and Explicit3.upl.
- Step 28 Keep the Output type as Grid for contouring.

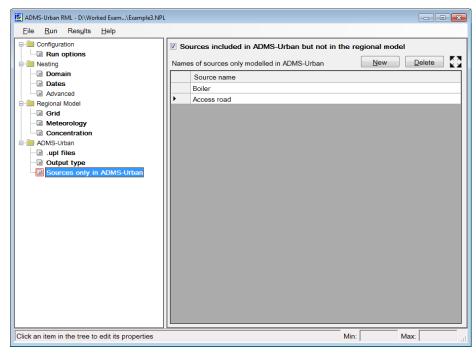


Figure 7.31 The list of Sources only in ADMS-Urban.

- Step 29 In the Sources only in ADMS-Urban section, select Sources included in ADMS-Urban but not in the regional model.
- Step 30 Click New twice, and enter the source names "Boiler" and "Access road".
- **Step 31** Save *Example3.npl* and then select **Run**, **Model**.

7.4.2 Analysing output

- Step 1 Start the COFP with the file *Example3.nc* loaded and open the **Create** Output Files screen.
- Step 2 Untick the Gridded Output option.
- **Step 3** Create a .pst file containing one hour average concentrations for all pollutants, as described in Section 7.2.2.

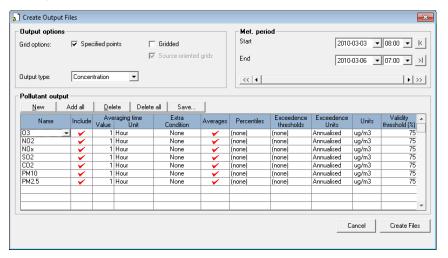


Figure 7.32 The COFP Create Output Files screen creating 1-Hour averages for specified points.

Step 4 Open *Example3.pst* in Excel and compare the output to that obtained in Example 1. Notice that the concentrations at the Roadside and Park monitors are the same, but that the concentrations at the Monastery monitor have increased.

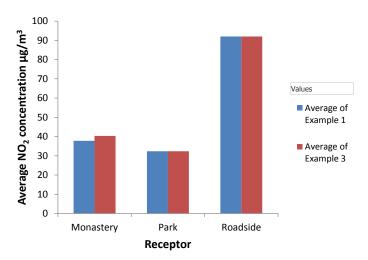


Figure 7.33 Comparing average concentrations at each receptor.

Step 5 In the COFP Create Output Files screen, create a .glt file containing Period averages for all pollutants for Gridded points and Source-oriented grids, as described in Section 7.3.2.

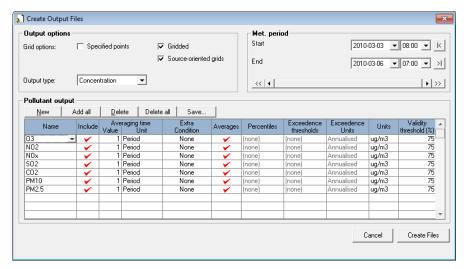


Figure 7.34 The COFP Create Output Files screen creating gridded period averages.

Step 6 In the ADMS Mapper, create contours of *Example3.glt*, as described in Section 7.3.3. Compare these contours to those created in Example 2. Notice that the newly added sources have slightly increased the local concentrations.

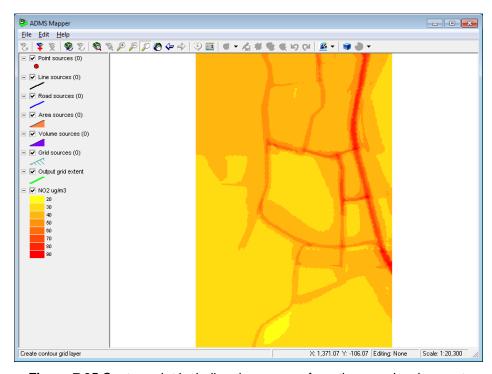


Figure 7.35 Contour plot including the sources from the new development.

SECTION 8 Technical Summary

This section gives technical information about the concept and implementation of the ADMS-Urban Regional Model Link (RML). The original concept of nesting ADMS-Urban within a regional model in order to model an urban area at all scales, with results from an initial implementation in London using CMAQ as the regional model, was published as Stocker *et al.* (2012). Further development of the concept was carried out using results from the EMEP4UK regional model in collaboration with researchers from the UK Centre for Ecology and Hydrology (CEH), supported by the UK Department of the Environment, Food and Rural Affairs (Defra). The development of the automated ADMS-Urban RML system was carried out using CAMx regional modelling in collaboration with researchers from the Hong Kong University of Science and Technology, supported by the Hong Kong Environmental Protection Department.

8.1 Concept

The concept of the ADMS-Urban RML system is based on a mixing time, T_m , defined as the length of time required after release for a plume from an explicitly-modelled source to be well-mixed on the scale of the regional model grid cells. For times longer than T_m after release, the regional model will give a good representation of dispersion and chemistry, whereas for the initial period, within T_m after release, a local model should be used to represent the detailed dispersion and chemistry. In general, T_m depends on the size of the regional model grid cells, the size and elevation of the explicitly modelled source, and the meteorological conditions. However, a fixed value of T_m of 1 or 2 hours has been found to be sufficient for modelling urban areas.

The theoretical expression for nested concentrations at an instantaneous output time t is as follows:

Nested receptor concentration

$$= RM(0:t) - RM(t - T_m:t) + ADMS-Urban expl (t - T_m:t)$$
 (1)

where the first term on the right hand side is the standard regional model (RM) concentration including emissions from all times up to t, the second is an adjustment to remove the regional model concentrations from emissions from times less than T_m prior to t, and the third is the replacement with ADMS-Urban concentrations from explicit modelling of emissions at times less than T_m before t.

In practice, it is difficult and computationally inefficient to modify and re-run the regional model to obtain the second term in (1) above, so this part of the expression is substituted with gridded emissions modelled in ADMS-Urban, giving the following expression:

Nested receptor concentration

$$= RM(0:t) - ADMS$$
-Urban grid $(t - T_m:t) + ADMS$ -Urban expl $(t - T_m:t)$

where

ADMS-Urban grid $(t - T_m: t)$ = the concentration field due to all emissions within the area of interest represented as gridded sources, dispersing from time t- T_m to time t = the concentration field due to all emissions within the area of interest represented at the highest known resolution, dispersing from time t- T_m to time t

ADMS-Urban with gridded sources can adequately represent the dispersion and chemistry of the regional model over the small temporal and spatial scales implied by the mixing time (T_m) in one grid cell. An ADMS-Urban grid run for one grid cell for a year takes around ten minutes of computer processing time, in contrast to months of computer processing time required to re-run a multi-scale regional model with modified emissions.

The ADMS-Urban calculations also use concentrations derived from the regional model as urban background boundary conditions, which are necessary for accurate calculations of local chemistry effects, and provide a further connection between the regional and local models in the ADMS-Urban RML system. Only one set of regional model data is required for this type of system, which reduces the computational resources required for its implementation.

The standard version of ADMS-Urban calculates 'steady-state' concentrations, by assuming that the concentrations at each hour are independent, and allowing emissions to disperse indefinitely. For nesting, an additional input option is specified in ADMS-Urban by the ADMS-Urban RML system so that the dispersion and chemistry calculations are truncated at a specified time, such as T_m . This option for temporal truncation of dispersion calculations is described in more detail in Section 8.5.1.2.

Only using regional model emissions from prior to T_m before the output time t (0: t - T_m), and local model emissions from after T_m before t (t - T_m : t) ensures that no double-counting of emissions can occur. Each model will satisfy conservation of mass, including dispersion and chemistry effects, for the subset of emissions that it includes, hence also ensuring overall mass conservation.

8.2 Implementation

The control program component of the ADMS-Urban RML Controller reads the information supplied by the user in the .npl file and automates a sequence of utility and ADMS-Urban runs. A nesting domain which covers multiple regional model grid cells is automatically divided into separate runs for each grid cell, with the results re-combined at the end of the ADMS-Urban RML system run. Template .upl input files for ADMS-Urban are supplied by the user, and the RML Controller substitutes appropriate meteorological and background concentration data files containing data from the corresponding regional model grid cell. The ADMS-Urban runs are initialised via CERC's Run Manager software, which allows them to be distributed across multiple PCs.

The main procedures included in the ADMS-Urban RML system for a run with output at a small number of receptor locations, suitable for model validation against measured data from specific monitoring sites, are shown as a flow chart in **Figure 8.1**. A brief description of each stage follows the diagram, while more details about the individual utilities can be found in the Appendices. Additional processes required to obtain output at a large number of locations,

Regional Model Meso-scale Key meteorological Concentration Utility data (WRF) output Data 1 Model run Meteorological Local upwind data for use in background ADMS-Urban ADMS-Urban Emissions data gridded run for background (1/2) 3 Nesting background ADMS-Urban ADMS-Urban Main gridded run (ΔT) Main explicit run (ΔT) Nested output = Regional Model concentrations - ADMS-Urban concentrations (gridded emissions, ΔT)

suitable for creating high-resolution contour plots, are described in Section 8.3.

Figure 8.1 Flow chart showing the main operations in the ADMS-Urban RML system. Each number, with associated green line(s), corresponds to a utility. Solid blue lines indicate meteorological data, dashed blue lines indicate emissions data and dotted blue lines indicate background concentration data.

+ ADMS-Urban concentrations (explicit emissions , ΔT)

Step 1 Initialisation of the ADMS-Urban RML system

The ADMS-Urban RML Controller control program reads the data from the .npl file and sets up the primary variables for the ADMS-Urban RML system run. In particular, it calculates the number and locations of the regional model grid cells which are included in the nesting domain, as most of the subsequent processes (Step 2 to Step 8) are replicated for each grid cell.

Step 2 ADMS-Urban runs for initial checking.

An initial set of ADMS-Urban runs are created using the .upl file with explicit emissions, truncated to each regional model grid cell included in the nesting domain and with the **Create ASP** mode selected, in order to check which cells contain output points. Any cells which do not contain any output points are excluded from further processing. Please refer to Section 8.5.1.3 for details of the ADMS-Urban **Create ASP** mode.

Step 3 Utility 1 - Extract meteorological data from WRF

The first utility used in the ADMS-Urban RML system is the utility for extracting meteorological data from WRF files. This utility is run for each grid cell to create an ADMS format met file (.met) for each cell, which is used for all subsequent ADMS-Urban runs in that cell. Details of this utility can be found in Appendix A.

Step 4 Utility 2 – Extract local upwind background concentrations

The second utility used in the ADMS-Urban RML system extracts local upwind background concentrations from the regional air quality model output files. These are defined as the concentrations from the neighbouring regional model cell in the upwind direction. The utility is run for each regional model grid cell included in the nesting domain and creates ADMS format background concentration files (.bgd).

Further details of the RML Background utility can be found in Appendix B. Note that the same utility is used for both the extraction of upwind background concentrations and the calculation of nesting background concentrations, with the required mode selected via the input file.

Step 5 ADMS-Urban run with gridded emissions

The first full ADMS-Urban model run in the ADMS-Urban RML system uses gridded emissions matched as closely as possible to the regional model emissions. The control program supplies file paths for the corresponding meteorology and background data files, and sets spatial and temporal truncation limits of the grid cell boundaries and half an hour, respectively. In general the ADMS-Urban grid source resolution will match the regional model grid resolution and one output point will be specified at the centre of each grid source cell, so the truncated runs will each contain only one grid source cell and one output point, leading to short run times.

The concentrations calculated by this run are relatively insensitive to both truncation time and averaging time, due to being output at the centre of the grid source. Further details of the user inputs to this run can be found in Section 4.4.1.1. The output from this run is an ADMS-Urban short-term specified point file (*.pst*).

Step 6 Utility 3 - Calculate nesting background concentrations

The third utility used in the ADMS-Urban RML system calculates the nesting background concentrations, defined as

Nesting background
$$= RM(0:t) - \left[ADMS-Urb \text{ grid}\left(t - \frac{1}{2}:t\right) - \text{local upwind background}\right]$$

where: 'RM(0:t)' is the regional model concentration in the relevant grid cell; 'ADMS-Urb grid $\left(t-\frac{1}{2}:t\right)$ ' is the output concentration from the ADMS-Urban run with gridded emissions matching the regional model emissions and dispersion truncated at half an hour (Step 5); and 'local upwind background' is the background concentration extracted in Step 4.

This nesting background concentration dataset represents the regional model (RM) concentration in the nesting domain throughout output hour by using the instantaneous value estimated at the middle of the output hour. The direct contribution of the nesting background to the final concentrations is zero, due to the subtraction of the gridded runs from the explicit runs, which both use the same nesting background. However, an appropriate value of nesting background is

important for accurate representation of the local chemistry processes.

Further details of the **RML Background** utility can be found in Appendix B. Note that the same utility is used for both the extraction of upwind background concentrations and the calculation of nesting background concentrations, with the required mode selected via the input file. The output from this utility is an ADMS format background concentration file (.bgd).

Step 7 Main ADMS-Urban runs

The main ADMS-Urban runs, with gridded and explicit emissions, are run using the regional meteorology extracted in Step 3 and the nesting background concentrations calculated in Step 6.

If a mixing time of more than one hour is used, separate model runs will be performed for each hour of the mixing time in order to take account of variations in emissions and background concentrations. When the output concentrations are combined:

- the output from the run with truncation from 0 to 1 hour is taken from the output hour,
- the output from the run with from 1 to 2 hours is taken from the hour before the output hour
- and so on for longer mixing times.

This ensures that appropriate time-varying emissions factors have been used. This approach assumes that meteorological conditions vary more slowly between hours than emission rates and background concentrations.

The runs with gridded and explicit emissions must include exactly the same output locations. Further details of the user inputs to these runs can be found in Sections 4.4.1.2 and 4.4.1.3. The outputs from these runs are ADMS Comprehensive Output File (COF) format netCDF files (.nc).

Step 8 Utility 4: Calculate nesting output concentrations

The fourth utility used in the ADMS-Urban RML system calculates nested concentrations, defined as follows:

$$C_N(t, \mathbf{X}_{OP})$$

$$= [S]C_{RM}(t, \mathbf{I}_{OP})$$

$$+ \sum_{i=1}^{T_M} C_{ADMS_{Ei}}(t-i+1, \mathbf{X}_{OP}) - \sum_{i=1}^{T_M} C_{ADMS_{Gi}}(t-i+1, \mathbf{X}_{OP})$$

where $C_N(t, \mathbf{X}_{OP})$ is the nested output concentration at time t (hours) and output point location \mathbf{X}_{OP} ; $[S]C_{RM}(t, \mathbf{I}_{OP})$ is the regional model concentration at time t and grid cell indices of the output point \mathbf{I}_{OP} , converted from regional model to ADMS speciation via the species map matrix [S]; T_M is the mixing time in integer hours; $C_{ADMS_{Ei}}(t-i+1,\mathbf{X}_{OP})$ is the concentration from ADMS-Urban run with

explicit emissions, truncated from $\tau = i - 1$ to $\tau = i$, at output time t - i + 1 and output point location X_{OP} ; and $C_{ADMS_{Gi}}(t - i + 1, X_{OP})$ is the concentration from ADMS-Urban run with gridded emissions, truncated from $\tau = i - 1$ to $\tau = i$, at output time t - i + 1 and output point location X_{OP} .

The utility is run for each regional model grid cell covered by the nesting domain. The output from this utility is an ADMS COF format netCDF file (.nc). Please refer to Appendix C for more information about the RML Output utility.

Step 9 Utility 5: Combine output files

The fifth utility used in the ADMS-Urban RML system combines the output concentration files from each regional model grid cell covered by the nesting domain into a single output file for the whole domain. The output from this utility is an ADMS COF format netCDF file (.nc). Please refer to Appendix D for more information about the **Combine COF** utility.

Step 10 Return final output and any required intermediate files to .npl directory

The ADMS-Urban RML Controller copies the final concentration output file, the RML Controller and other RML system component log files and any additional files requested by the user to the original .npl file directory.

8.3 Additional RML system procedures for high-resolution contour output

When ADMS-Urban is run as a stand-alone model for high-resolution contours of concentration, three types of output locations are included in the final .gst or .glt files:

- a regular grid of output points which provide the underlying grid resolution away from explicitly modelled sources;
- primary source-oriented grid points, which are added to increase the resolution where
 the highest concentration gradients are expected, such as along explicitly modelled
 roads, and which are included in the main concentration calculations; and
- secondary or interpolated intelligent grid points, which are inserted in between pairs of primary source-oriented grid points at the end of the run and given concentrations interpolated between the adjacent modelled concentrations.

This combination of output point types helps to generate smooth concentration contours at high resolution without requiring excessive modelling calculations. In order to allow the same type of high resolution contour output from the ADMS-Urban RML system, two procedures are required in addition to those described in Section 8.2, firstly to define a consistent set of output points for the main nesting runs with and without explicit emissions, and secondly to add interpolated intelligent grid points to the final output.

8.3.1 Defining output point locations: ADMS-Urban Create ASP mode

Instead of Step 2 of the main RML system procedures described in Section 8.2, the .upl with explicit emissions is run with spatial truncation to the whole nesting domain,

using the ADMS-Urban **Create ASP** mode, in order to generate an Additional Specified Points (*.asp*) file containing any specified points, the regular grid points and the primary source-oriented grid points for the whole nesting domain. Please refer to Section 8.5.1.3 for more details of the ADMS-Urban **Create ASP** mode.

Creating the .asp file for the whole nesting domain rather than for individual regional model grid cell regions allows high-resolution contours to be created across the boundaries between regional model grid cells, which are otherwise run independently in the RML system.

8.3.2 Adding interpolated concentrations

The **AddInterpIGP** utility is run after the nested concentration files have been combined for the whole nesting domain in Step 9. This ensures that pairs of source-oriented grid points which lie on different sides of a boundary between adjacent regional model grid cells can be used to create interpolated source-oriented grid points. The output from this utility is an ADMS COF format netCDF file (.nc), with the points reclassified as regular or source-oriented grid points as appropriate. Please refer to Appendix E for more information about the **AddInterpIGP** utility.

8.4 Treatment of sources only included in ADMS-Urban

The ADMS-Urban RML system is designed to allow some sources only to be included in the ADMS-Urban modelling, for example if the emissions associated with a new or proposed development were not included in the regional modelling. These sources require special treatment for two reasons:

- their emissions should not be included in either of the .upl files with gridded emissions which are used to imitate the regional model behaviour, as they were not included in the regional model; and
- temporal truncation should not be applied to the ADMS-Urban dispersion calculations, as the long-range dispersion of their emissions will not be modelled by the regional model.

The user is required to define their .upl emissions to satisfy the first condition, while the RML Controller handles the second condition. If the mixing time is defined as one hour, sources not included in the regional model emissions are run without truncation in the ADMS-Urban run with explicit emissions. If the mixing time is defined as longer than one hour, the explicit .upl is run multiple times for each regional model grid cell covered by the nesting domain, each time with different temporal truncation limits covering each hour of the mixing time. Sources which are only included in ADMS-Urban are run without truncation in one of these runs, and excluded from the other runs, to avoid multiplying their emissions. Please refer to Section 8.5.1.2 for more details of the temporal truncation of dispersion in ADMS-Urban.

8.5 Components of the ADMS-Urban RML system

The ADMS-Urban RML Controller coordinates a series of ADMS-Urban model runs, submitted via Run Manager, and utility programs. Some of the ADMS-Urban and Run Manager features used in the ADMS-Urban RML system are specific to this system, so may not be described in their respective User Guides. Section 8.5.1 covers the key ADMS-Urban features used in the ADMS-Urban RML system and Section 8.5.2 the Run Manager automation functions. The RML Controller utility programs are described in the Appendices to this User Guide.

8.5.1 ADMS-Urban model options

For details of the spatial truncation of dispersion, chemistry schemes and standard dispersion of individual source emissions, please refer to the main ADMS-Urban User Guide.

8.5.1.1 .umo model override files

A .umo file contains a subset of the information found in an ADMS-Urban model parameter (.upl) file, and is used to replace definitions found in the original .upl. For example, the ADMS-Urban RML Controller uses .umo files to specify appropriate .met, .bgd and .uai files for each regional model grid cell, without needing to edit the template .upl. Any input section of the .upl file structure which is not repeated can be overridden using a .umo file. For example, this means that meteorological or output settings can be changed but source and pollutant data cannot be redefined.

If a .umo file has been used, the ADMS-Urban .log file will include the statement:

```
INFO : A ^{\star}.umo file has been used to overwrite the original model set up
```

All contents of the .log file will reflect the settings and file paths specified in the .umo file, where relevant. The .umo file must have the same file-name stem as the .upl and be saved in the same directory, with the .umo extension. For example, if the template .upl is saved as $D:\My\ Work\Test.upl$ then a .umo file would have to be saved as $D:\My\ Work\Test.umo$ in order to be used.

Note that a .uai file path specified in a .umo file will replace any .uai file specified in the original .upl.

8.5.1.2 Temporal truncation of dispersion

A key part of the ADMS-Urban RML system concept is that the regional model modelling is used to represent dispersion over long time-scales, while ADMS-Urban modelling is used for short time-scales. When ADMS-Urban is run as a stand-alone model, it calculates dispersion of emissions separately for each hour and allows the emissions from that hour to disperse for all time. When used in the RML system, however, the ADMS-Urban model calculations must be restricted to short time-scales using an additional input option for temporal truncation.

The ADMS-Urban temporal truncation option is controlled by an additional input file (.uai) section. Both lower and upper time thresholds can be specified, as this is necessary when a mixing time of more than one hour is specified, to allow runs to be divided into single hour sections of the mixing time.

Sources not requiring temporal truncation, for example those not included in the regional modelling, can be listed. If the run is specified as 'primary' – by convention, with a lower temporal truncation threshold of zero – excluded sources will be modelled by the standard ADMS-Urban method with no truncation. If the run is 'secondary' – by convention, with a lower temporal truncation threshold greater than zero – excluded sources will not be modelled. Hence when a mixing time greater than one hour is used, sources excluded from truncation will be modelled in full in the run with truncation from 0 to 1 hour, but not modelled in the run(s) with truncation from 1 to 2 hours or later. This treatment ensures that the effects of emissions from sources not included in the regional modelling are included in full but without double-counting in the final results.

When the temporal truncation option is in use, and some sources are being excluded from truncation, the log file from a primary run will include the following statements:

```
Dispersion time truncation in use, limits 0.00 to 1.00 hours

Primary run for partial dispersion time truncation, excluded sources will be modelled for all times

The following sources are excluded from dispersion time truncation:

example road2
```

8.5.1.3 Create ASP mode

The **Create ASP** mode of ADMS-Urban is specified as an additional input (.uai file) option. When this option is specified, the model reads all source data, identifies all output locations including any source-oriented grid points, and writes an additional specified points file (.asp) which includes all the output locations with unique names. The output point naming convention is related to the type and locations of the points, which are used by the utility to add interpolated intelligent grid points, as described in Appendix E. The output file is saved in the same directory as the .upl file, with the same file-name stem and the extension .out.asp. No meteorological pre-processing or dispersion calculations are performed in this mode.

The **Create ASP** mode will take account of any intelligent grid point settings included in an .igp file, as specified in a .uai file for the run with explicit emissions. For example, the maximum number of primary intelligent grid points can be increased, the spacing between points adjusted and certain sources excluded from source-oriented points. Please refer to the ADMS-Urban user guide section 'Source-oriented grids' for more information about the .igp file options and format.

The naming conventions used by the **Create ASP** mode in ADMS-Urban are as follows:

- Any user-defined specified output points retain their original names.
- The regular grid points are given names which indicate their type and their

position in the regular grid point sequence, for example |G|0000001 for the bottom left hand corner of the grid.

- The primary source-oriented grid points for road and line sources (intelligent grid points) are given names which indicate their type and their 'pairing' to another point for the purposes of interpolating secondary intelligent grid points, for example |I|000001_P000005 for the first primary intelligent grid point which forms a pair with the fifth primary intelligent grid point. If the option to omit interpolated intelligent grid points is selected in an .igp file, the 'pairing' information will not be included in the names given to the primary intelligent grid points.
- The source-oriented grid points for point, area and volume sources (nested points) are given names which indicate their type and the name of the source with which they are associated, for example |N|StackA for a nested grid point associated with the 'StackA' source.

Please refer to the ADMS-Urban user guide 'Source-oriented grids' section for more information about the different types of source-oriented grid points and interpolated intelligent grid points.

The use of "|" characters in the point names, which are banned from use in the ADMS-Urban interface and hence cannot occur in user-specified output point names, ensures that the names given to the grid points cannot conflict with those of user-defined output points.

The .uai file section for using the Create ASP mode has the following format:

CREATEASP Y

8.5.2 Run Manager options

Run Manager is generally used to coordinate ADMS runs from multiple users across one or more runs machines. Users submit, monitor, collect and delete runs using the Run Manager interface. In the ADMS-Urban RML system, these functions have been automated.

The use of Run Manager in the RML system allows ADMS-Urban runs to be distributed for execution across a group of runs machines, which enables multiple runs to be performed simultaneously. This allows the RML system to model large nesting domains containing multiple regional model cells efficiently, as the ADMS-Urban runs required for each cell and hour of the mixing time can be processed independently.

Please refer to the Run Manager User Guide (CERC, 2014b) for details of the standard use of Run Manager.

8.5.2.1 Automation of submitting, collecting and deleting runs

The RML Controller interacts with Run Manager functions without using the Run Manager interface. It submits ADMS-Urban runs to the Run Manager central

repository using the Model and Execution Group settings specified in the .npl file. The priority of the runs is set to a standard value, which can be altered by editing the RML configuration file.

Machines within the specified Run Manager Execution Group with spare capacity for ADMS-Urban runs look for waiting runs in the central repository, transfer the files and executable to their local working directory and perform the run. While the run is in progress, the executing machine issues status updates to the central repository so the run progress can be monitored by the RML Controller. When the run is complete, the executing machine returns the run files to the central repository. The RML Controller collects the files and deletes the run from the central repository.

The user can monitor the progress of the RML runs using the **Run Status** screen in the Run Manager interface, which will show both RML runs and any stand-alone ADMS-Urban runs submitted manually to Run Manager.

The location of the Run Manager central repository must be defined in the RML Controller configuration file to enable the interaction between the RML Controller and Run Manager. An installation of Run Manager on the same machine as the RML Controller is useful for allowing the user to monitor run progress, but not required, and as this installation is unlikely to be used to execute runs, it does not need to be licensed.

8.6 ADMS-Urban RML System limits

8.6.1 Permitted characters

Only characters which are defined within the Windows setting of "Language for non-Unicode programs" (code page or system locale) may be used within the ADMS-Urban RML Controller interface. For example, if your "Language for non-Unicode programs" is "English (United Kingdom)", selecting a file path for the species map file from the RML Controller interface which contains Chinese characters will create a corrupt species map file path when the *.npl* file is saved.

If you need to transfer .npl and/or .upl files between computers with different settings of "Language for non-Unicode programs", only basic latin characters and punctuation (ASCII characters 1-127) should be used in file paths and within text files, to ensure compatibility.

Please refer to Microsoft advice on "Changing the system locale" for further information.

8.6.2 Numbers of sources

The numbers of explicit and gridded sources defined in the .upls input to the ADMS-Urban RML system may be very large, to include all sources within the urban area of

http://windows.microsoft.com/en-gb/windows/change-system-locale#1TC=windows-7

interest. The maximum number of each source type which can be defined in the ADMS-Urban interface is 100000 road sources, 10000 industrial sources and 100000 grid source cells.

The number of explicit and gridded sources which can be included in each regional model grid cell within the nesting domain is controlled by the terms of your ADMS-Urban license.

8.6.3 Options not included in final RML system output

User-defined group output and deposition rates are not currently included in the final RML system output files. These options may still be specified in the RML system .upls, for example to take account of the plume depletion caused by deposition, or for investigations of the contributions of different source types in the explicitly-modelled ADMS-Urban concentrations.

8.6.4 Options not permitted in RML system input .upls

The **Odours**, **Buildings** and **Aircraft Sources** options must not be included in any of the RML system input .upls.

SECTION 9 References

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APPENDIX A WRF to Met utility

The WRFtoMet utility is a command line application which extracts meteorological data from WRF netCDF files and creates ADMS format .met files. It was developed for the ADMS-Urban RML system but may also be useful for generating .met files for stand-alone ADMS-Urban modelling runs. Please refer to the WRF model documentation (Skamarock et al., 2008) for details of the WRF variables and output file format.

A.1 Data requirements

The WRF output files must each contain one hour of data, and have file names and/or directory structures which indicate the date and time of the data they contain. This enables the utility to generate the file path for the file containing a specific hour of data from the supplied templates. The period over which meteorological data is required may span many WRF files, but they should all have the same file-name pattern, differing only in date and time values.

The WRF output files must contain at least the following attributes or variables:

- Latitude and Longitude;
- Map projection type;
- Simulation start time;
- Wind speeds at 10 m (U10, V10) or at grid heights; and if the latter, also terrain heights, base-state and perturbation geopotentials; and
- At least one of incoming solar radiation and surface sensible heat flux.

Some other requirements depend on the type of coordinates used to specify the location at which meteorological data should be extracted from WRF output: if grid indices are used, no additional information is required and no additional restrictions are applied to the choice of coordinate system. If lat-long or projected coordinates are used, the following additional requirements apply:

- The map projection type must be Lambert Conformal Conic or Polar Stereographic;
- The appropriate parameters for a full definition of the projected coordinate system must be present as attributes.

A.2 Processing assumptions

The meteorological data saved to WRF output files is instantaneous, giving a snapshot of the meteorological conditions at that particular time. For the purposes of using WRF data in ADMS, it is assumed to represent the overall met conditions for the previous hour, hence matching the hour-ending ADMS convention.

The WRFtoMet utility will always extract data from the lowest grid layer, except if the U10,

V10 option for wind speeds is selected, in which case the wind speed and direction will be extracted from the values at 10 m. The height at which the wind speed was extracted is written to the header of the .met output file. At present the utility does not create a profile file containing meteorological data at multiple heights.

The WRFtoMet utility extracts most WRF variables with the assumption that their units in WRF are the same as those required in ADMS, so does not perform any unit conversions, except for temperature where a conversion from Kelvin to Celsius is required. The units assumed in WRF and required in ADMS for the variables extracted by the WRFtoMet utility are listed in **Table A.1**.

The precipitation variables in WRF store cumulative values of precipitation, whereas ADMS uses hourly rates of precipitation. The WRFtoMet utility converts WRF precipitation to hourly rates by subtracting the previous hour's cumulative precipitation from the current hour. This requires all WRF files to be derived from the same WRF run, and for one hour of data to be available immediately before the first extracted hour. Note that precipitation rates are only used by ADMS-Urban if wet deposition calculations are required.

WRF met variable	WRF unit assumed	ADMS met file unit
Wind speeds	ms ⁻¹	ms ⁻¹
Temperature (2m)	K	°C
Heights	m	m
Solar radiation	Wm ⁻²	Wm ⁻²
Heat flux	Wm ⁻²	Wm ⁻²
Precipitation	mm (cumulative)	mm (per hour)
Geopotentials	m^2s^{-2}	m^2s^{-2}

Table A.1 The units used in ADMS-Urban and assumed for WRF output files for selected meteorological variables

A.3 Input file format

The input file for the WRFtoMet utility is a text file, which must have the file name "WRF Input.txt" and be saved in the same folder as the WRFtoMet executable.

The input file contains five sections. The start of a section is denoted by an ampersand ('&') and the section name, while the end of a section is denoted by a forward slash ('/'). Each variable within a section must be on a separate line, and text entries should be delimited by inverted commas (''). The sections must be listed in the order given below, but the variables within each section may be specified in any order.

The WRF_FileAttributes section contains information about the location(s) of the WRF files that will be used in the utility run. All the entries in this section must be completed.

The WRF_TableNames section contains information about the names of the WRF variables from which you wish to extract data. You do not have to include variable names for meteorological data you do not wish to extract. If a variable name for a variable you wish to extract does not exist in the WRF file then the utility will stop with an error. However, if a variable name for a variable which exists in the file but is not the intended variable is

specified, the data values are within the valid ranges allowed by ADMS and the variable dimensions are the same as those expected, the utility will extract the values from the named variable. Therefore it is important to ensure that the specified variable names correspond to the appropriate variables.

The WRF_UseTables section contains information about which meteorological variables you wish to extract. If any of the categories are not included in the input file then data will not be extracted from the relevant variables.

The WRF_DimAttNames section contains the names of the required WRF variables and attributes. All the entries in this section must be completed.

The WRF_TimeInfo section contains information about the time structure of the WRF output files. All the entries in this section must be completed.

Tables **A.2** to **A.6** list all the available options for each section with descriptions and comments. An example file is shown in **Figure 9.1**, and a default template is included in the ADMS-Urban RML installation directory, by default *<install_path>\Data*. Note that the RML Controller will overwrite the values of the variables in the WRF_FileAttributes and WRF_TimeInfo sections using data from the RML Controller interface, so the template file does not include entries for these sections.

If you wish to extract precipitation data from WRF, the WRF file from the hour before the specified start time must be available and all of the WRF files must be output from the same WRF simulation. If the initial WRF file is missing, the utility run will stop with an error and no .met file will be created. If the WRF files are not all from the same WRF run a warning will be issued and a .met file will be created without precipitation data.

Figure 9.1 Example WRFtoMet input file

Variable name	Required	Description	Comment
WRF_Directory	Y	Date-independent directory path for WRF output files	Please refer to Section 4.3.2.2 for more details of the
WRF_FilePattern	Y	Date and time-dependent file and/or folder pattern for WRF output files	directory path and file name template specification of regional model file paths

Table A.2 Variables in the WRF_FileAttributes section of the WRFtoMet input file

Variable name	Required	Description	Comment	
WRF_Name_WindU10	N	WRF variable name for West-East wind speeds at 10 m	Must both be included if using	
WRF_Name_WindV10	N	WRF variable name for South-North wind speeds at 10 m	WRF_Use_Wind10	
WRF_Name_WindU	N	WRF variable name for West-East wind speeds at all heights		
WRF_Name_WindV	N	WRF variable name for South-North wind speeds at all heights	Must all be included if using	
WRF_Name_TerrHgt	N	WRF variable name for terrain heights	WRF_Use_WindHgts	
WRF_Name_GeopotBase	N	WRF variable name for base-state geopotentials		
WRF_Name_GeopotPert	N	WRF variable name for perturbation geopotentials		
WRF_Name_TempT2	N	WRF variable name for temperature at 2 m	Must be included if using WRF_Use_TempT2	
WRF_Name_BLayerHgt	N	WRF variable name for boundary layer height	Must be included if using WRF_Use_BLayerHgt	
WRF_Name_SolarRad	N	WRF variable name for incoming solar radiation	Must be included if using WRF_Use_SolarRad	
WRF_Name_HeatFlux	N	WRF variable name for surface sensible heat flux	Must be included if using WRF_Use_HeatFlux	
WRF_Name_CumRain	N	WRF variable name for cumulative cumulus (subgrid scale) precipitation	Must both be included if using	
WRF_Name_GridRain	N	WRF variable name for cumulative grid-scale precipitation	WRF_Use_Rain	

Table A.3 Variables in the WRF_TableNames section of the WRFtoMet input file. WRF_Use_* variables are included in the WRF_UseTables section of the input file and are in use if set to .TRUE.

Variable name	Required	Description	Comment
WRF_Use_Wind10	N	Extract wind speed and direction from the values at 10 m	One of WRF_Use_Wind10 and
WRF_Use_WindHgts	N	Extract wind speed and direction from the lowest grid layer data	WRF_Use_WindHgts must be .TRUE.
WRF_Use_TempT2	N	Extract values of temperature at 2 m	
WRF_Use_BLayerHgt	N	Extract values of boundary layer height	
WRF_Use_SolarRad	N	Extract values of incoming solar radiation	At least one of WRF_Use_SolarRad
WRF_Use_HeatFlux	N	Extract values of surface sensible heat flux	and WRF_Use_HeatFlux must be .TRUE.
WRF_Use_Rain	N	Extract values of precipitation	

Table A.4 Variables in the WRF_UseTables section of the WRFtoMet utility input file. Each of these variables may be set to .TRUE. or .FALSE.

Variable name	Required	Description	Comment
WRF_DimAttName_EastWest	Y	WRF East-West dimension name	
WRF_DimAttName_NorthSouth	Y	WRF North-South dimension name	
WRF_DimAttName_BottomTop	Y	WRF vertical dimension name	
WRF_DimAttName_TimeDim	Y	WRF time dimension name	Time dimension: number of time-steps included in the file
WRF_DimAttName_Longitude	Y	WRF Longitude variable name	
WRF_DimAttName_Latitude	Y	WRF Latitude variable name	
WRF_DimAttName_Times	Y	WRF Time variable name	Time variable: value of date/time at each time-step
WRF_DimAttName_MapProj	Y	WRF map projection attribute name	
WRF_DimAttName_RefLong	Y	WRF reference longitude attribute name	
WRF_DimAttName_RefLat	Y (LCC)	WRF reference latitude attribute name	Parameters used to describe the map
WRF_DimAttName_StdPar1	Y	WRF first standard parallel attribute name	projection for coordinate transformations
WRF_DimAttName_StdPar2	Y (LCC)	WRF first standard parallel attribute name	
WRF_DimAttName_SimStartTime	Y	WRF simulation start time attribute name	

Table A.5 Variables in the WRF_DimAttNames section of the WRFtoMet input file. The map projection attributes are only required if lat-long or projected coordinates are used for specifying the input location. (LCC) in the 'Required' column indicates that this parameter is only required for the Lambert Conformal Conic projection.

Variable name	Required	Description	Comment
WRF_TimeBetweenFiles _Hrs	Y	Number of whole hours between consecutive WRF files	
WRF_TimeDiff_UTCtoL ocal_Hrs	Y	Number of whole hours between UTC and local time	For example, 0 for UK, -5 for New York and +8 for Hong Kong

Table A.6 Variables in the WRF_TimeInfo section of the WRFtoMet input file

A.4 Command line structure

The following command line arguments are required to run the WRFtoMet utility:

```
[exe name] yyyy mm dd hh ll output met name coord flag x coord y coord
```

Where:

- [exe_name] is the full file-path to the WRFtoMet executable, enclosed in inverted commas ('').
- yyyy is the year of the first date for which met data should be extracted, in local time.
- mm is the month of the first date for which met data should be extracted, in local time.
- dd is the day of the month of the first date for which met data should be extracted, in local time.
- hh is the hour the first date for which met data should be extracted, in local time.
- 11 is the number of hours of met data which should be extracted.
- output_met_name is the file path and name of the output met file, enclosed in inverted commas ('').
- coord_flag is a flag which identifies the form of the input coordinates. One of the following numerical values should be specified:
 - * 0 to use WRF grid indices;
 - * 1 to use latitude-longitude coordinates in units of decimal degrees; or
 - * 2 to use projected coordinates in units of metres.
- x_coord is the x-coordinate of the point for which met data should be extracted. Its
 value will depend on the coordinate system being used, corresponding to the value of
 the coord_flag as follows:
 - * 0 x-direction (west-east) WRF grid index;
 - * 1 longitude coordinate; or
 - * 2 x-direction (west-east) projected coordinate.
- y_coord is the y-coordinate of the point for which met data should be extracted. Its
 value will depend on the coordinate system being used, corresponding to the value of
 the coord_flag as follows:
 - * 0 y-direction (south-north) WRF grid index;
 - * 1 latitude coordinate; or
 - * 2 y-direction (south-north) projected coordinate.

For example, if the utility executable is saved in the default installation directory, $C:\Program\Files\(x86)\CERC\RML$, and meteorological data is required from 9am on 1st January 2010 for 5 days, for the grid cell with index values (3,4), with output to be saved in the file $D:\My\Work\WRF_output.met$, the command line should be:

```
'C:\Program Files (x86)\CERC\RML\WRFtoMet.exe' 2010 01 01 09 120
```

```
'D:\My Work\WRF output.met' 0 3 4
```

Note that the start date and time is specified in local time, as used in ADMS-Urban. Specifying coordinate values which are outside the WRF domain will cause the utility to stop with an error. It may be easiest to specify the command line arguments via a batch file (.bat).

A.5 Utility outputs

The WRFtoMet utility creates a single ADMS format .met meteorological data file containing the variables selected in the input file over the period specified in the command line, from all the relevant WRF output files. The utility will create a new file or overwrite any existing file which is located in the same directory and has the same name. It does not append data to an existing .met file.

A header section indicates when the file was created, the location where the meteorological data was extracted in the input location specification (projected or longitude/latitude coordinates) and grid index values, and the height corresponding to the wind speed and direction values. An example output file created by the WRFtoMet utility is shown in **Figure 9.2**.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the utility executable and input file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

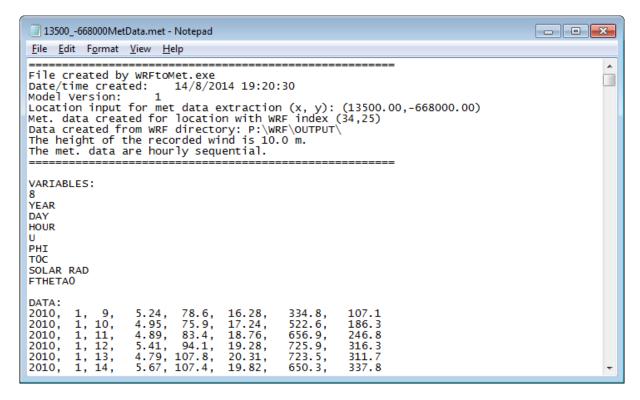


Figure 9.2 Example .met file produced by the WRFtoMet utility, viewed in Notepad

APPENDIX B RML Background utility

The **RML Background** utility is a command line application which creates ADMS-format .bgd files from regional air quality model concentrations. It has two modes:

- to calculate local upwind background concentrations, which is an angular average of concentrations from cells immediately upwind of the area of interest, and
- to calculate nesting background concentrations, which represent the concentration in the area of interest during the modelling time.

The utility was developed for use in the ADMS-Urban RML system, but the local upwind mode may also be useful for stand-alone runs of ADMS-Urban if rural monitoring data are not available outside the modelling area. Within the ADMS-Urban RML system, the **RML Background** utility is run separately for each regional model cell included in a larger nesting domain, but for a stand-alone utility run it could be used with a domain covering multiple regional model cells.

The **RML Background** utility is able to read concentrations from regional model output files from the CMAQ, CAMx (converted into IOAPI format) or EMEP4UK models. Output from any other model which can be manipulated to comply with the Models-3 I/O API netCDF Gridded file conventions (Coats, 2004) may also be used by selecting the CMAQ option.

B.1 Local upwind mode

The local upwind mode of the RML Background utility is illustrated in Figure 9.3. The utility interpolates between concentrations found at the centres of two regional model cells immediately outside the nesting domain and lying on each side of a line running upwind from the centre of the nesting domain, with weighting dependent on the wind direction.

The regional model concentrations are always read from the lowest vertical layer of the regional model grid. The processing domain must be entirely within the regional model horizontal grid extent, with a border of at least one cell in each direction, to allow the adjacent upwind cells to be used.

The utility uses a species map to convert from regional model chemical species to ADMS chemical species, please refer to Section 4.3.3.6 for more details of the species map concept and format. The output .bgd file concentration units are always written as ug/m3 so the species map factors must include a conversion from regional model units to $\mu g/m^3$, if required.

The utility reads an ADMS-format .met file to identify the wind direction for each hour in order to find the upwind cells. The .met file must include year, day, hour and wind direction variables, with any of the permitted ADMS variable names, and should be in local time.

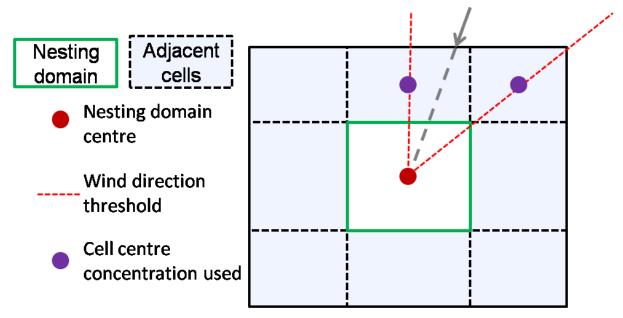


Figure 9.3 Diagram of the local upwind background mode of the **RML background** utility. The output background concentration is interpolated between the upwind cell concentrations according to the wind direction.

B.2 Nesting background mode

The nesting background mode of the **RML Background** utility calculates nesting background concentrations, defined as

Nesting background
$$= RM(0:t)$$

$$- \left[ADMS-Urb \text{ grid} \left(t - \frac{1}{2}:t\right) - \text{local upwind background}\right]$$

where:

- 'RM' is the average regional model concentration in the lowest layer from the grid cells within the nesting domain;
- 'ADMS-Urb grid $\left(t \frac{1}{2} : t\right)$ ' is the output concentration from the ADMS-Urban run with gridded emissions matching the regional model emissions and dispersion truncated at half an hour (Step 5 in the description of the RML system procedures in Section 8.2); and
- 'local upwind background' is the background concentration extracted in Step 4.

This nesting background represents the regional model (RM) concentration in the nesting domain throughout the mixing time by using the instantaneous value estimated at the middle of the mixing time.

The utility reads the local upwind .bgd file and the .pst file output from the ADMS-Urban run with gridded emissions. Both are required to contain concentrations in $\mu g/m^3$ units for the ADMS species listed in the species map file. The output .bgd file concentration units are always written as $\mu g/m^3$ so the species map factors must include a conversion from regional

model units to µg/m³, if required.

The .pst file can include one or more receptors within the nesting domain. If more than one receptor is located in the nesting domain and listed in the input file, the .pst concentrations from all the listed receptors are averaged when calculating the nesting background concentrations. When used in the ADMS-Urban RML system, the .pst file is expected to include one receptor in the centre of each regional model grid cell, but the RML Controller will include any receptors found within the cell.

If the nesting domain includes multiple regional model cells, the concentrations from each cell included in the nesting domain are averaged when calculating the nesting background concentrations.

If a negative nesting background concentration is calculated for any ADMS species at any hour, the output concentration of that species is set to zero for that hour. The total number of hours with negative nesting background concentrations for any pollutant is written to a warning file at the end of the utility run. If the number of hours with negative nesting background is greater than 1% of the total number of hours included in the run, this may indicate a discrepancy in magnitude and/or time-variation between the regional model and ADMS-Urban emissions, which should be investigated. Common causes for negative nesting background concentrations are described in Section 6.7.6.

B.3 Input file format

The input file for the RML Background utility is a text file which contains a version string and three sections of data. The first two sections, whose elements are defined in **Table B.1**, are common to both modes of the program, whereas the keyword and contents of the third section, defined in **Table B.2**, control which mode of the program will be run. The order of the sections and the variables within each section must be as defined in **Tables B.1** and **B.2**. Each element should be given on a new line; blank lines may be included before each section keyword but not within a section. An example input file is shown in **Figure 9.4**.

The nesting domain should cover a whole number of regional model grid cells to within a tolerance of 10% of the regional model grid spacing. The nesting domain may cover any rectangular area of grid cells, it is not required to be square.

Element type	Description	Example entry	Comment
Version string	File version description	RMLBGDINPUTVERSION1	Must be the first line of the file
Section keyword	Start of section containing variables common to both modes	SHAREDRMLINPUTS	Also used in the RML Output utility, must be included
Variable	Regional model name	CMAQ	CMAQ, CAMx or EMEP4UK
Variable	Start date-time	2010,01,01,01	format YYYY, MM, DD, HH (year, month, day
Variable	End date-time	2010,12,31,24	of month, hour)
Variable	File path to species map file	PATH="D:\RML\SpeciesMap.csv"	Refer to Section 4.3.3.6 for details of the species map file format
Variable	File path to date-independent directory containing regional model output file	PATH="D:\CMAQ\Output"	
Variable	File name template for regional model output files	'%Y%M\cctm.%Y%M%D.nc'	Refer to Section 4.3.2.2 for details of the file name template tags
Variable	Number of hours in each regional model output file	24	
Variable	Time difference between local solar time and regional model time	1	Time difference in whole hours, can be positive or negative
Section keyword	Start of section defining nesting domain	NESTINGDOMAIN	Must be included
Variable	Type of nesting domain definition	INDICES	COORDS or INDICES
Variable	Central x coordinate (m)	18500	Included if the nesting domain type is COORDS
Variable	Central y coordinate (m)	-676000	
Variable	Domain extent in x-direction (m)	1000	
Variable	Domain extent in y-direction (m)	1000	
Variable	Lower left cell x index (column)	10	Included if the nesting domain type is INDICES
Variable	Upper right cell x index (column)	11	
Variable	Lower left cell y index (row)	15	
Variable	Upper right cell y index (row)	15	
Variable	Index of the grid layer nearest to the ground	1	

Table B.1 Specification of compulsory elements of the input text file format for the RML Background utility

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Element type	Description	Example entry	Comment
Section keyword	Start of section defining local upwind mode inputs	LOCALUPWINDBACKGROUND	Included for the local upwind mode only
Variable	File path of the output .bgd file	PATH = "D:\RML\upwind.bgd"	
Variable	File path of the input ADMS-format .met file	PATH = "D:\RML\WRFmet.met"	
Section keyword	Start of section defining nesting background mode inputs	NESTINGBACKGROUND	Included for the nesting background mode only
Variable	File path of the output .bgd file	PATH = "D:\RML\nesting.bgd"	
Variable	File path of the upwind .bgd file	PATH = "D:\RML\upwind.bgd"	
Variable	File path of the input .pst file	PATH = "D:\RML\NestBgd.pst"	
Variable	Number of .pst receptors to include in the calculations	1	
Variables	Names of <i>.pst</i> receptors to include in the calculations	Centre_1	List receptor names as used in ADMS, one per line, must be within the nesting domain

Table B.2 Specification of optional elements for the input text file of the **RML Background** utility. Note that one of the local upwind and nesting background mode sections must be included in the file.

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Figure 9.4 Example input file for the RML background utility viewed in Notepad

B.4 Command line structure

To run the **RML Background** utility from the command line or a batch file, the following syntax should be used:

```
<executable file path> <input text file path>
```

where <executable file path> is the full path to the utility executable (.exe), enclosed in inverted commas, and <input text file path> is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default RML Controller installation directory, $C:\Program\ Files\ (x86)\CERC\RML\$, and the input text file is saved as $D:\My\ Work\RMLBgdInput.txt$, the command line to run the utility would be

```
'C:\Program Files (x86)\CERC\RML\RMLBackground.exe' 'D:\My Work\RMLBqdInput.txt'
```

B.5 Utility outputs

The RML Background utility creates an ADMS format .bgd file containing background concentrations for the output species defined in the species map file, for the period specified in the input file if sufficient data are available, in units of $\mu g/m^3$. This utility will create a new .bgd file. It will stop with an error if an existing file is found with the same file path as specified for the output file, ie. it will not overwrite or append to an existing file.

A header section specifies when the file was created, in which mode the utility was run and the file path of the input text file used. An example output .bgd file is shown in **Figure 9.5**.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to

fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

Figure 9.5 Output .bgd file produced by the **RML Background** utility viewed in Notepad

APPENDIX C RML Output utility

The RML Output utility is a command line application which calculates nesting output concentrations from ADMS and regional model outputs and writes them to an ADMS format netCDF file. This utility was developed for use in the ADMS-Urban RML system and is specific to this system. Within the RML system, the utility is run separately for each regional model grid cell covered by the nesting domain, but it could be run for a larger domain if required.

C.1 Nesting output calculations

The RML Output utility calculates nested concentrations, defined as follows:

$$C_{N}(t, \mathbf{X}_{OP}) = [\mathbf{S}]C_{RM}(t, \mathbf{I}_{OP}) + \sum_{i=1}^{T_{M}} C_{ADMS_{Ei}}(t - i + 1, \mathbf{X}_{OP}) - \sum_{i=1}^{T_{M}} C_{ADMS_{Gi}}(t - i + 1, \mathbf{X}_{OP})$$

where $C_N(t, X_{OP})$ is the nested output concentration at time t (hours) and output point location X_{OP} ; $C_{RM}(t, I_{OP})$ is the regional model concentration at time t and grid cell indices of the output point I_{OP} ; [S] is the species map matrix used to convert from regional model to ADMS speciation; T_M is the mixing time in integer hours; $C_{ADMS_{Ei}}(t-i+1, X_{OP})$ is the concentration from ADMS-Urban run with explicit emissions, truncated from $\tau = i - 1$ to $\tau = i$, at output time t - i + 1 and output point location X_{OP} ; and $C_{ADMS_{Gi}}(t-i+1, X_{OP})$ is the concentration from ADMS-Urban run with gridded emissions, truncated from $\tau = i - 1$ to $\tau = i$, at output time t - i + 1 and output point location X_{OP} .

The ADMS-Urban concentrations are read from ADMS Comprehensive Output Files (netCDF format) and the calculated nested concentrations are written to a new netCDF file in the same format. The ADMS-Urban concentration datasets are required to have units of $\mu g/m^3$ and an averaging time of 1 hour. The utility will use concentrations only from the first group found in the Comprehensive Output File, which will be the 'All sources' group.

All the ADMS-Urban output files are required to contain the same output locations in the same order. This is usually achieved by using the same .asp file to specify output point locations for all runs. The horizontal extents of the nesting domain are calculated based on the output locations contained in the ADMS-Urban files. The vertical layer of the regional model grid matching each output location is calculated as specified in Section C.2. All output locations must be within the horizontal and vertical extents of the regional model grid, and are not required to form a rectangular area.

C.2 Calculation of Regional Model output heights

Most regional meteorological and air quality models run with vertical grid structure defined by pressure (sigma) coordinates, whereas ADMS-Urban uses absolute heights above ground level in metres. The conversion from sigma values to heights in general requires knowledge of the terrain height, which can vary in space, and the surface temperature and pressure, which can vary in both space and time.

Within the **RML Output** utility, heights are calculated from sigma values using the simplified 'reference state' assumptions with constant surface temperature and pressure, and assuming a constant terrain height. This is based on the approach used in the MM5 meteorological model (Dudhia *et al.*, 2005), which was a precursor to the WRF model. It avoids the need to re-read all the WRF data purely to obtain the regional model grid heights, and enforces constant grid heights, both of which speed up the processing time for the utility. The conversion of pressure coordinates to heights is more sensitive to the value of temperature than the value of terrain height, such that the use of a user-specified typical temperature and zero terrain height gives sufficient accuracy for the grid heights.

The expression used to calculate height from a sigma coordinate value σ is as follows:

$$z = -\frac{RA}{2g} \left(\left(\ln \left(\frac{(p_0 - p_T)\sigma + p_T}{p_0} \right) \right)^2 + \frac{2T_0}{A} \ln \left(\frac{(p_0 - p_T)\sigma + p_T}{p_0} \right) \right)$$

where: z is height above ground in metres; R is the gas constant for air (287 J/kgK); A is an atmospheric lapse rate (50 K); g is gravitational acceleration (9.81 m/s²); p_0 is the standard atmospheric pressure at sea-level (1.013x10⁵ Pa); p_T is the pressure at the top of the model grid, which may be obtained from the concentration output files or specified by the user; and T_0 is the standard temperature at sea-level in Kelvin, which is specified by the user.

C.3 Input file format

The input file for the RML Output utility is a text file which contains a version string and two or three sections of data. Two sections are compulsory and the third, which contains advanced parameters, is optional. The compulsory sections are described in **Table C.1** and the optional section in **Table C.2**. The 'SHAREDRMLINPUTS' section is identical to that used in the RML Background utility. The sections may be listed in any order but the order of the variables within each section must be as defined in **Tables C.1** and **C.2**. Each element should be given on a new line, blank lines may be included before each section keyword but not within a section. If the optional section is included, all the Y/N elements must be included, with values for any 'Y' elements. An example input file is shown in **Figure 9.6**.

If the mixing time is greater than one hour, the ADMS-Urban output files must be listed in descending order of truncation time, ie. the file from the run with truncation time from (mixing time -1) to (mixing time) is listed first, and the file from the run with truncation time from 0 to 1 last. For example, if a mixing time of three hours was in use, the list of output files from runs with gridded emissions should be:

MainGrid truncation2 3.nc

MainGrid_truncation1_2.nc
MainGrid truncation0 1.nc

Figure 9.6 Example input file for the RML output utility

Element type	Description	Sample element	Comment
Version string	File version description	'RMLINPUTVERSION1'	Must be the first line of the file
Section keyword	Start of section containing general variables	'SHAREDRMLINPUTS'	Also used in the RML Background utility,
Variable	Regional model name	CMAQ	must be included. Please refer to Table B.1 for details
Variable	Start date-time	2010,01,01,01	B.1 for details
Variable	End date-time	2010,12,31,24	
Variable	File path to species map file	PATH="D:\RML\SpeciesMap.csv"	
Variable	File path to date-independent directory containing regional model output file	PATH="D:\CMAQ\Output"	
Variable	File name template for regional model output files	'%Y%M\cctm.%Y%M%D.nc'	
Variable	Number of hours in each regional model output file	24	
Variable	Time difference between local solar time and regional model time	1	
Section keyword	Start of section with variables specific to RML output	'RMLOUTPUT'	Must be included
Variable	File path of output netCDF file	PATH="D:\RML\Output.nc"	
Variable	Mixing time in whole hours	1	
Variable	List of file paths for gridded nesting run output files	PATH="D:\RML\MainGrd.nc"	If mixing time is greater than one, must be listed with decreasing truncation time
Variable	Mixing time in whole hours	1	Must be the same as above
Variable	List of file paths for explicit nesting run output files	PATH="D:\RML\MainExplicit.nc"	If mixing time is greater than one, must be listed with decreasing truncation time

Table C.1 Specification of elements which must be included in the input file for the RML Output utility

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Element type	Description	Sample element	Comment
Section keyword	Start of optional section containing advanced settings	'ADVANCEDNESTING'	May be omitted
Variable	Whether to specify frequency of checking output point locations match	'Y'	Y or N
Variable	frequency of checking output locations match	5	only included if Y above, default value 1
Variable	Whether to specify sea-level temperature	'Y'	Y or N
Variable	Average sea-level temperature in Kelvin	298	only included if Y above, default value 288.15
Variable	Whether to override the model top pressure	'Y'	Y or N
Variable	Model top pressure in Pascals	5000	only included if Y above, default to use the value from the regional model concentration output files

Table C.2 Specification of optional advanced settings which may be included in the input file for the RML Output utility

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C.4 Command line structure

To run the **RML Output** utility from the command line or a batch file, the following syntax should be used:

```
<executable file path> <input text file path>
```

where <executable file path> is the full path to the utility executable (.exe), enclosed in inverted commas, and <input text file path> is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default RML Controller installation directory, $C:\Program\ Files\ (x86)\CERC\RML\$, and the input text file is saved as $D:\My\ Work\RMLOutputInput.txt$, the command line to run the utility would be

```
'C:\Program Files (x86)\CERC\RML\RMLOutput.exe' 'D:\My
Work\RMLOutputInput.txt'
```

C.5 Utility outputs

The RML Output utility writes output concentrations to a netCDF (.nc) file which follows the ADMS Comprehensive Output File conventions. This format is described in full in the ADMS-Urban User Guide. This utility will always create a new .nc file - it will stop with an error if an existing file is found with the same file path as specified for the output file, so it will not overwrite or append to an existing file.

Descriptive attribute values are copied from the first ADMS-Urban input file, while the concentration datasets are defined according to the ADMS species specified in the species map file. The netCDF data contents can be viewed and processed using the ADMS Comprehensive Output File Processor utility.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX D Combine COF utility

The **Combine COF** utility is a command line application which combines ADMS Comprehensive Output Files (netCDF) for different spatial and/or temporal modelling regions into a single file in the same format. This utility was developed for the ADMS-Urban RML system and for the parallel development of a system to distribute runs in a cloud computing environment. It may be useful for recombining output files if a large stand-alone ADMS-Urban run has been divided into multiple time periods or multiple spatial regions to allow efficient use of computing resources.

D.1 Data requirements

The input netCDF files may contain data for different spatial regions, different time periods or both, with the following restrictions:

- If there are different time-periods, they must form an uninterrupted hourly sequence;
- If there are different spatial regions and different time-periods, the same spatial split between files must be maintained for all time-periods, ie. the file for region 1 must contain the same output points during all time periods; and
- The spatial regions must be exclusive, so there is no duplication of output point names.

The full set of output locations are included in the output netCDF file, this may include any combination of specified points, regular grids and/or source-oriented grids. The utility will reorder the gridded output points to fit the ADMS-Urban Comprehensive Output File conventions.

If gridded output points are included in the input files, the utility can check whether they form a regular rectangle with consistent x and y coordinates in order to output a valid grid. If the gridded output points do not form a complete rectangular grid, there is an option for them to be converted into specified point outputs.

D.2 Input file format

The components of the input text file for the **Combine COF** utility are defined in **Table D.1**. There is only one section in the input file for this utility. An example input file is shown in **Figure 9.7**.

The **Combine COF** utility can treat output points in two different ways, either as their original types (specified point, gridded or source-oriented), including checks for the consistency of gridded output locations and retaining the user-specified point names; or all as specified points, with numerical names. The 'Receptor option' element in the input file should be set to Y for the first method or N for the second method.

Element type	Description	Example element	Comment
Version string	File version description	CombineCOFVersion1	Must be the first line of the file
Section keyword	Start of section with input data	COMBINECOF	Must be included
Variable	Output file path	PATH="D:\RML\Combined.nc"	
Variable	Whether multiple time- periods are included	'Y'	Y or N
Variable	Number of time-periods	2	Only included if Y above, must be greater than 1
Variable	Whether multiple spatial regions are included	'Y'	Y or N
Variable	Number of spatial regions	2	Only included if Y above, must be greater than 1
Variable	Receptor option	'Y'	Y to check grid, N to convert all points to receptors
Variable	Total number of input netCDF files	4	Number of time- periods*number of spatial regions
Variable	List of netCDF file paths	PATH="D:\RML\Region1Time1.nc" PATH="D:\RML\Region2Time1.nc" PATH="D:\RML\Region1Time2.nc" PATH="D:\RML\Region2Time2.nc"	Must list all spatial files for the same time period together, and spatial regions in the same order for all time periods, with time periods in chronological order

 $\textbf{Table D.1} \ \textbf{Specification of input file format for the } \textbf{Combine COF} \ \textbf{utility}$

```
CombineCOFInput.txt - Notepad

File Edit Format View Help

COMBINECOFVERSION1
COMBINECOF
PATH="D:\RML-System\Working\CombineCOF.nc"
N
Y
3
Y
3
PATH="D:\RML-System\Working\-3500_-665000\-3500_-665000RMLoutput.nc"
PATH="D:\RML-System\Working\-3500_-664000\-3500_-664000RMLoutput.nc"
PATH="D:\RML-System\Working\-2500_-663000\-2500_-663000RMLoutput.nc"
```

Figure 9.7 Example input text file for the Combine COF utility

D.3 Command line structure

To run the **Combine COF** utility from the command line or a batch file, the following syntax should be used:

```
<executable file path> <input text file path>
```

where <executable file path> is the full path to the utility executable (.exe), enclosed in inverted commas, and <input text file path> is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default installation directory, $C:\Program\ Files$ $(x86)\CERC\RML\$, and the input text file is saved as $D:\My\ Work\CombineCOFInput.txt$, the command line to run the utility would be

```
'C:\Program Files (x86)\CERC\RML\CombineCOF.exe' 'D:\My Work\CombineCOFInput.txt'
```

D.4 Utility outputs

The **Combine COF** utility writes output concentrations to a netCDF (.nc) file which follows the ADMS Comprehensive Output File conventions. This format is described in full in the ADMS-Urban User Guide. The utility will overwrite any existing file with the specified output file name and location.

Descriptive attribute values, such as the **Site Name**, are copied from the first input netCDF file. The netCDF data contents can be viewed and processed using the ADMS Comprehensive Output File Processor utility.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX E AddInterplGP utility

The AddInterpIGP utility is a command-line application which adds interpolated intelligent grid points to an input ADMS-format netCDF file. This utility was developed for use in the ADMS-Urban RML system but may also be useful when stand-alone ADMS-Urban modelling of high-resolution concentration contours is required over a large area. It allows the runs to be divided into smaller spatial regions for more efficient use of available computing resources and later re-combined without loss of contour resolution at the boundaries of the smaller regions. Please refer to the **Source-oriented grids** section of the ADMS-Urban User Guide for more details about intelligent grid points and interpolated intelligent grid points.

E.1 Data requirements

The AddInterpIGP utility reads an ADMS-format netCDF file, which must contain output from an ADMS-Urban run where the output locations were defined by an .asp file created using the Create ASP mode of ADMS-Urban (as described in Section 8.5.1.3). Further specified points may have been defined in the .upl of the run using the .asp file, but no gridded output should have been included. This ensures that the output locations in the netCDF file have the names required to allow the AddInterpIGP utility to determine where to locate interpolated intelligent grid points, and to re-convert gridded output locations from specified points to gridded points.

If the runs using the .asp file have been split into multiple spatial regions and the output netCDF files re-combined using the **Combine COF** utility, the order of the .asp points in the final output file may not match that in the original .asp file. The **AddInterpIGP** utility will reorder the points before the calculations of interpolated point locations and concentrations.

E.2 Interpolation of concentrations

The **AddInterpIGP** utility uses the same method for determining the locations and output concentrations for interpolated intelligent grid points as used by ADMS-Urban for a standalone run with source-oriented gridding for road and line sources. Please refer to the Source-oriented grids section of the ADMS-Urban User Guide for more details.

E.3 Input file format

The **AddInterpIGP** utility does not use an input text file.

E.4 Command line structure

To run the AddInterpIGP utility from the command line or a batch file, the following syntax should be used:

<executable file path> <input COF file path> <output COF file path>

where: <executable file path> is the full path to the utility executable (.exe), enclosed in inverted commas; <input COF file path> is the full path to the input Comprehensive Output File (.nc) to which interpolated source-oriented grid points should be added, enclosed in inverted commas; and <output COF file path> is the full path to the output Comprehensive Output File (.nc) including interpolated source-oriented grid points, enclosed in inverted commas. The output file path may be omitted, in this case the utility will create a file with the same file stem and location as the input file but with the .out.nc extension.

For example, if the executable is saved in the default installation directory, $C:\Pr or Files(x86)\setminus CERC\setminus RML\setminus$, and the input netCDF file is saved as $D:My\ Work\setminus ContourOutput.nc$, the minimum command line to run the utility would be

```
\label{lem:contour} $$ 'C:\Pr GPam Files (x86)\CERC\RML\AddInterpIGP.exe' `D:\My Work\ContourOutput.nc'
```

and in this case the output file would be saved as $D:My\ Work\setminus ContourOutput.out.nc$.

E.5 Utility outputs

The **AddInterpIGP** utility writes output concentrations for all input grid locations and added interpolated intelligent grid points to a netCDF (.nc) file which follows the ADMS Comprehensive Output File conventions. This format is described in full in the ADMS-Urban User Guide. The utility will overwrite an existing file with the specified output file name and location, but the output file path cannot be the same as the input file path.

Descriptive attribute values, such as the **Site Name**, are copied from the input netCDF file. The netCDF data contents can be viewed and processed using the ADMS Comprehensive Output File Processor utility.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input netCDF file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.



Cambridge Environmental Research Consultants Ltd 3 King's Parade, Cambridge, CB2 1SJ, UK Tel: +44 (0)1223 357 773, Fax: +44 (0)1223 357 492

Email: help@cerc.co.uk Website: www.cerc.co.uk